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HPC Software – Compiler and Tools

May 2015 | Michael Knobloch

Outline

Make it work,
make it right,
make it fast.

Kent Beck

- Local module setup
- Compilers*
- Libraries*

Debuggers:
- STAT
- TotalView
- MUST

Performance Tools:
- Score-P
- Scalasca
- Vampir
- HPCToolkit
- Performance Reports
- TAU

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Module setup & compiler

The Module Setup

- Tools are available through “modules”
  - Allows to easily manage different versions of programs
  - Works by dynamic modification of a user's environment

- JUQUEEN: Module setup based on UNITE
  - Tools only visible after a `module load UNITE`
  - User has to take care of dependencies

- JUROPATEST: Module setup based on EasyBuild and lmod
  - Staged, hierarchical setup
  - Automatically manages dependencies via toolchains

Most Important Module Commands

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module

- `spider` # lmod only: show all products
- `spider` *`product`* # lmod only: show product details
- `avail` # show all available products
- `list` # list loaded products

- `load` *`product(s)`* # setup access to product
- `unload` *`product(s)`* # release access
- `swap` *`product1 product2`* # replace v1 of product with v2

- `whatis` *`product(s)`* # print short description
- `help` *`product(s)`* # print longer description
- `show` *`product(s)`* # show what “settings” are performed

Compiler and MPI libraries

- JUQUEEN
  - IBM XL C/C++ and Fortran compiler
  - GNU C/C++ and Fortran compiler
  - Clang C/C++ compiler
  - IBM MPI
- JUROPATEST
  - Intel C/C++ and Fortran compiler
  - GNU C/C++ and Fortran compiler
  - Intel MPI
  - Parastation MPI

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Debuggers

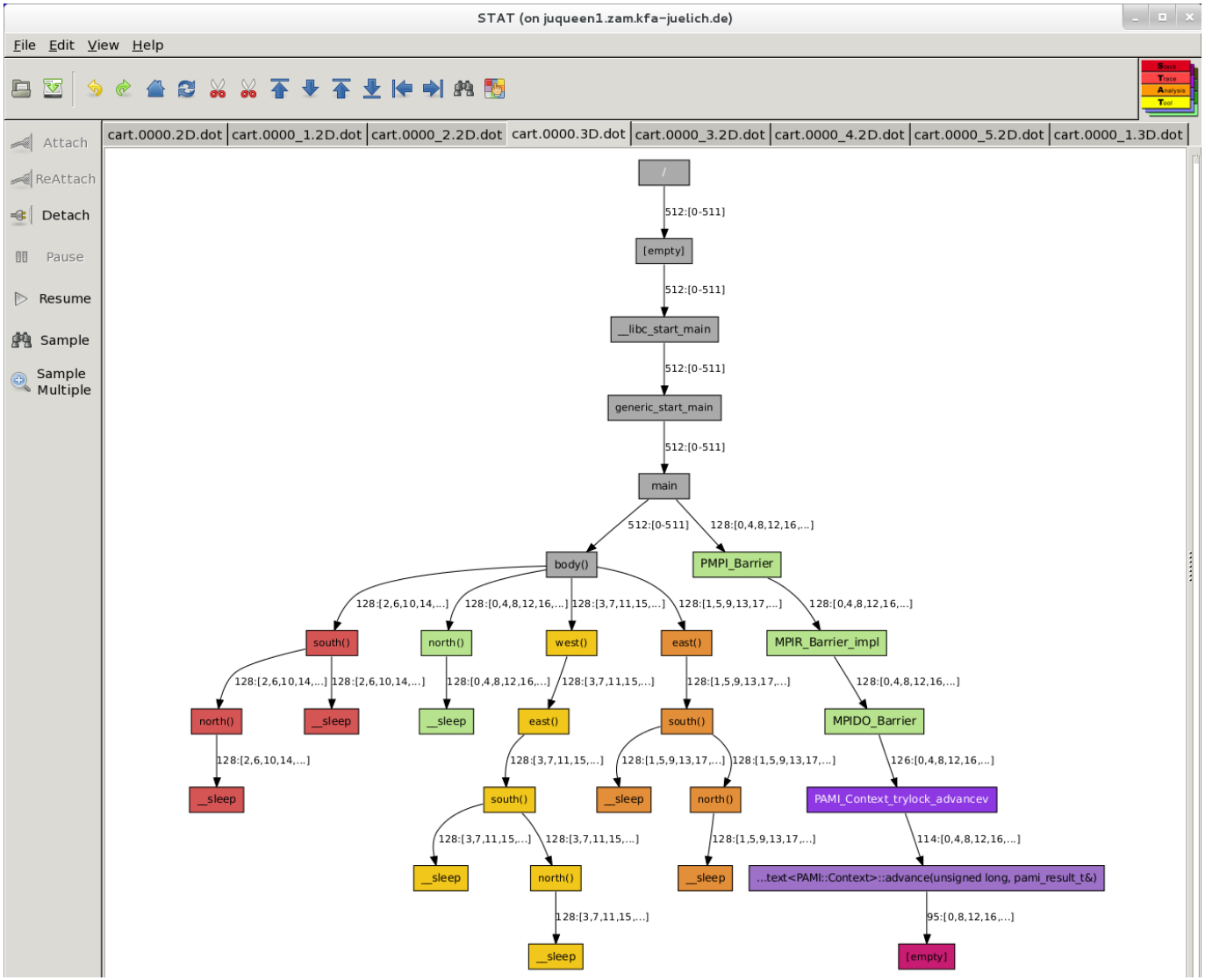
Debugging Tools (status: May 2015)

	JUQUEEN	JUROPATEST
Debugging		
STAT	✓	(×)
TotalView debugger	✓	✓
MUST MPI verification tool	✓	(×)
DDT debugger*	×	(×)

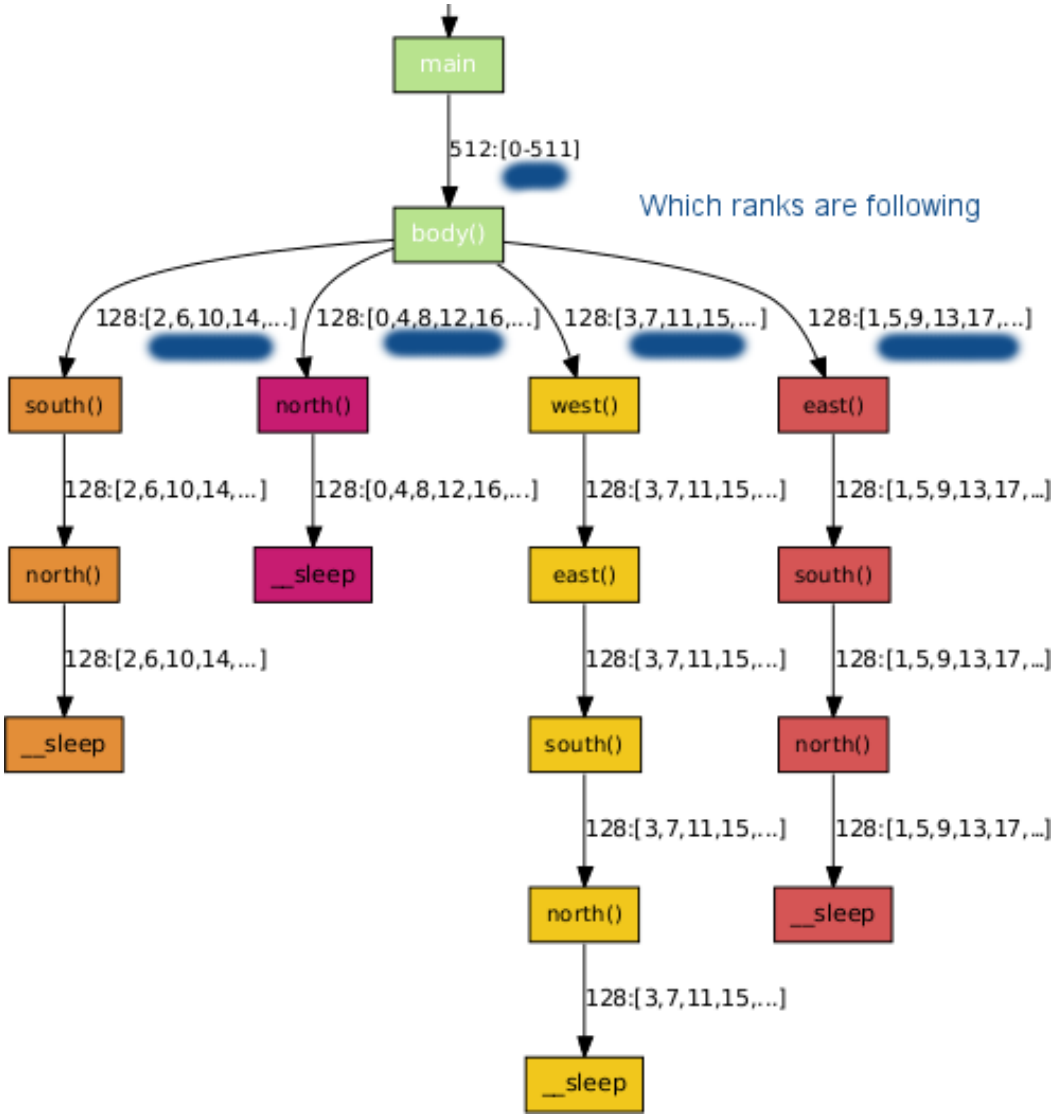
STAT: Stack Trace Analysis Tool

- Very lightweight helper tool
- Shows merged call tree of whole program
- Useful to detect deadlocks
- Scales to millions of processes
  - http://www.hpcwire.com/hpcwire/2012-12-03/bug_repellent_for_supercomputers_proves_effective.html
- Pinpoint individual problems
- **NOT** a real/full debugger
- http://www.paradyn.org/STAT/STAT.html

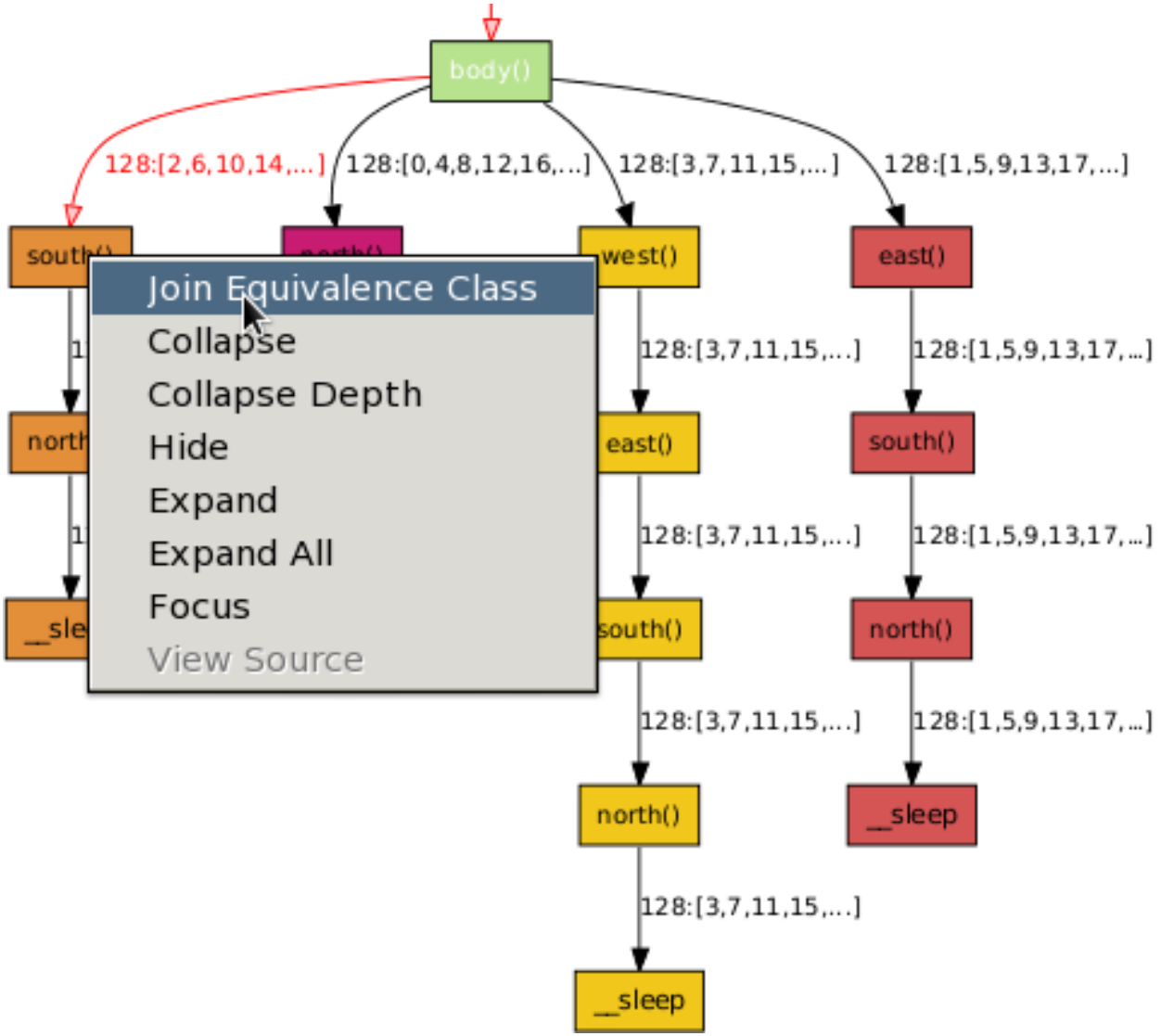
STAT: Main Window



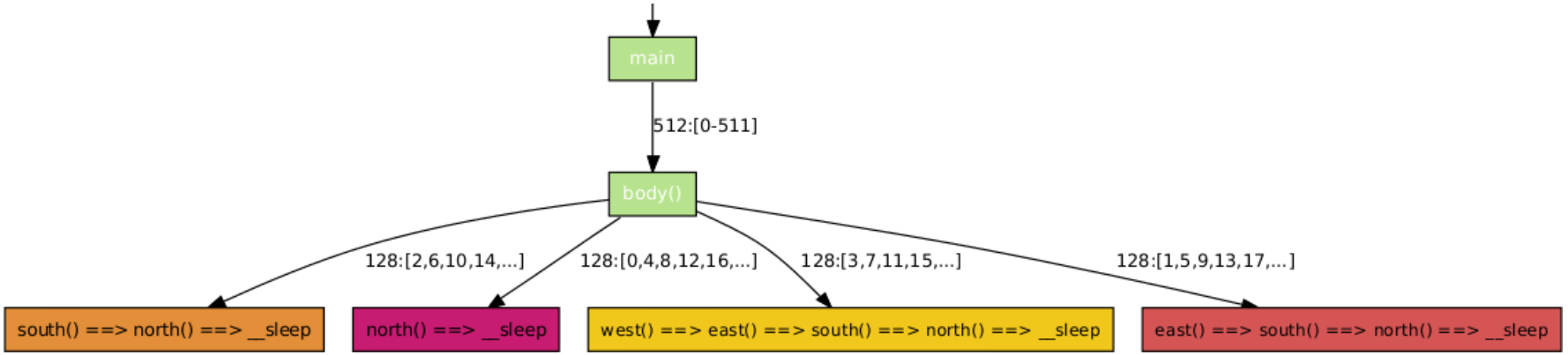
STAT: Zoom


main
512:[0-511]
Which ranks are following
body()
128:[2,6,10,14,...]
128:[0,4,8,12,16,...]
128:[3,7,11,15,...]
128:[1,5,9,13,17,...]
south()
north()
west()
east()
128:[2,6,10,14,...]
128:[0,4,8,12,16,...]
128:[3,7,11,15,...]
128:[1,5,9,13,17,...]
north()
__sleep
east()
south()
128:[2,6,10,14,...]
128:[3,7,11,15,...]
128:[1,5,9,13,17,...]
__sleep
south()
north()
128:[3,7,11,15,...]
128:[1,5,9,13,17,...]
north()
__sleep
128:[3,7,11,15,...]
__sleep

STAT: Equivalence Classes



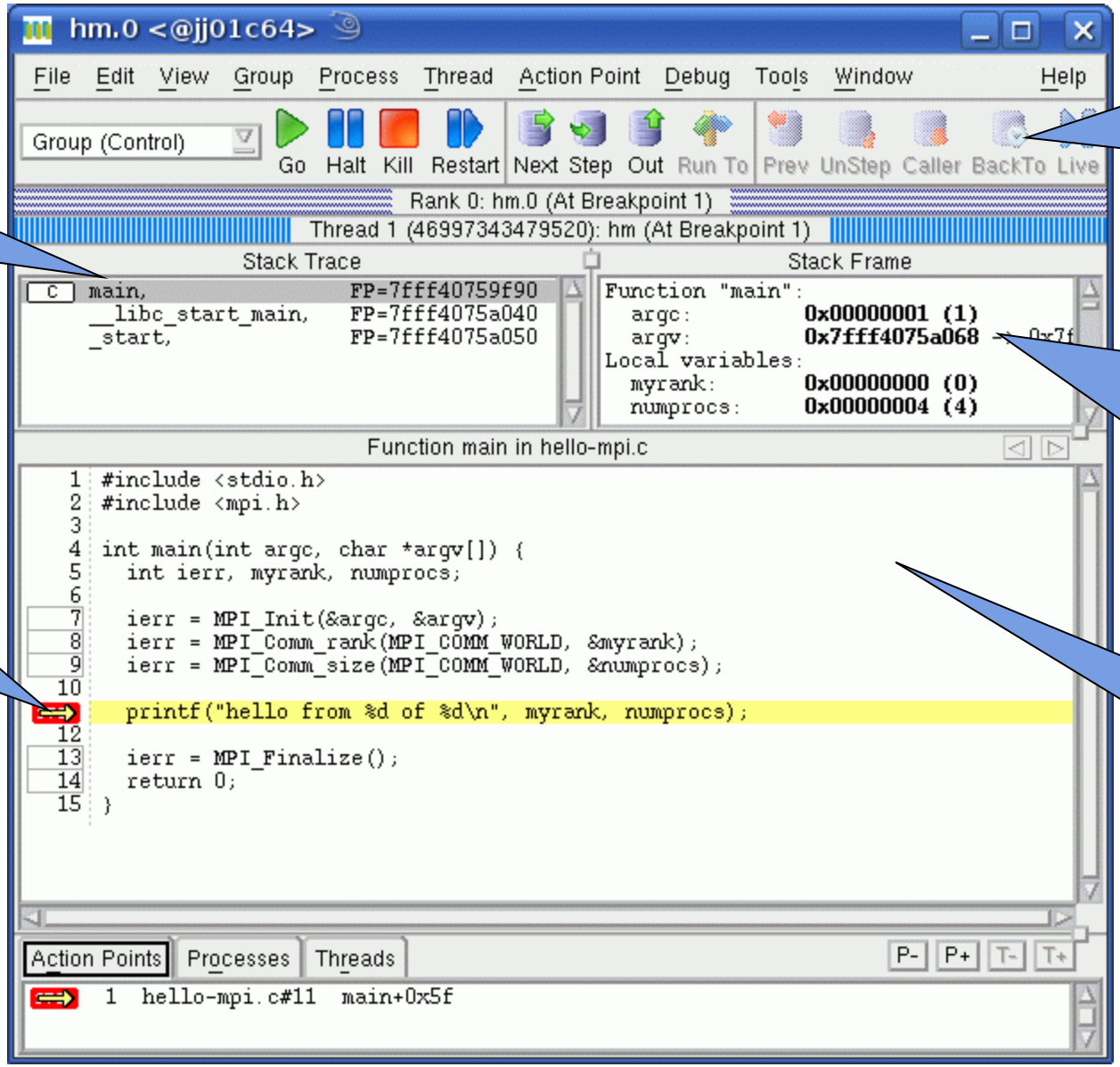
STAT: Equivalence Classes (cont.)



Parallel Debugger

- UNIX Symbolic Debugger
  for C, C++, F77, F90, PGI HPF, assembler programs
- “Standard” debugger
- Special, non-traditional features
  - Multi-process and multi-threaded
  - C++ support (templates, inheritance, inline functions)
  - F90 support (user types, pointers, modules)
  - 1D + 2D Array Data visualization
  - Support for parallel debugging (MPI: automatic attach, message queues, OpenMP, pthreads)
  - Scripting and batch debugging
  - Memory Debugging
- http://www.roguewave.com
- NOTE: License limited to 2048 processes (shared between all users)

TotalView: Main Window



Stack trace

Toolbar for common options

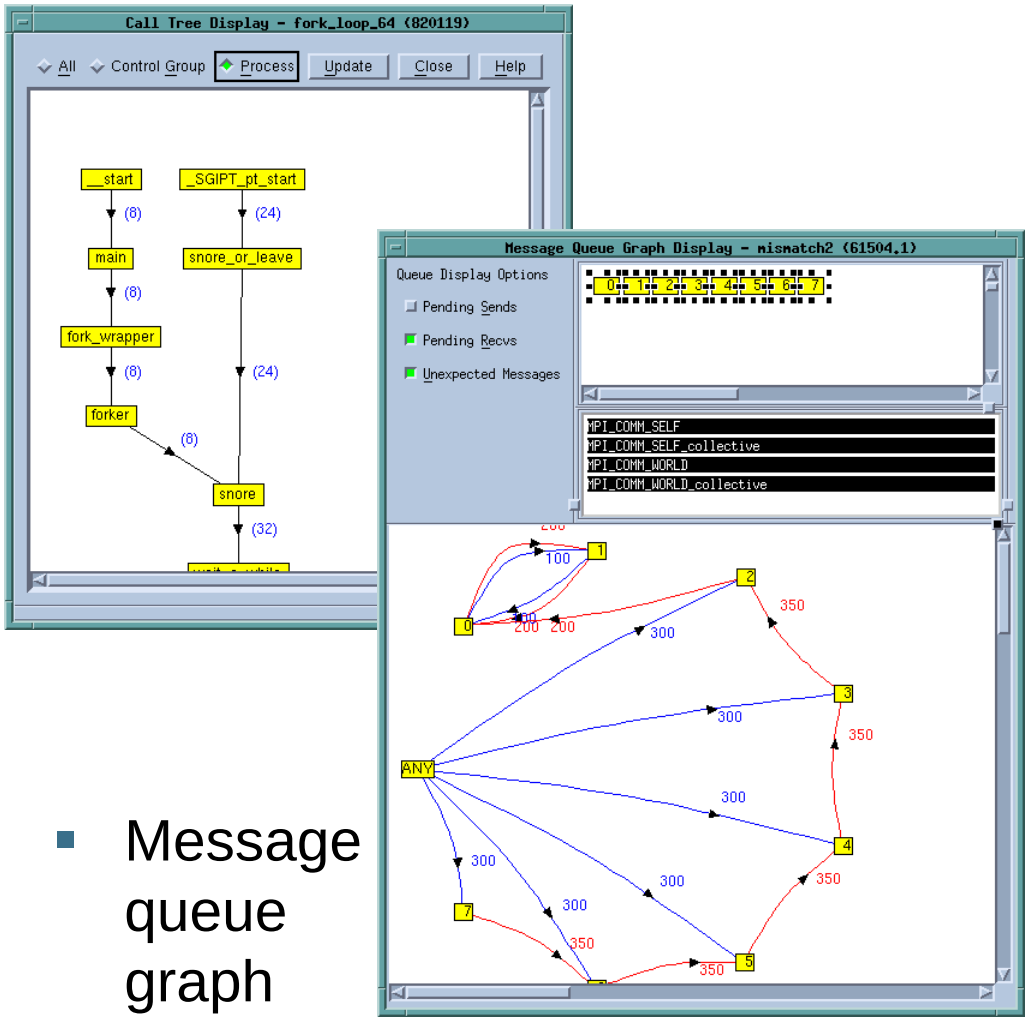
Local variables for selected stack frame

Break points

Source code window

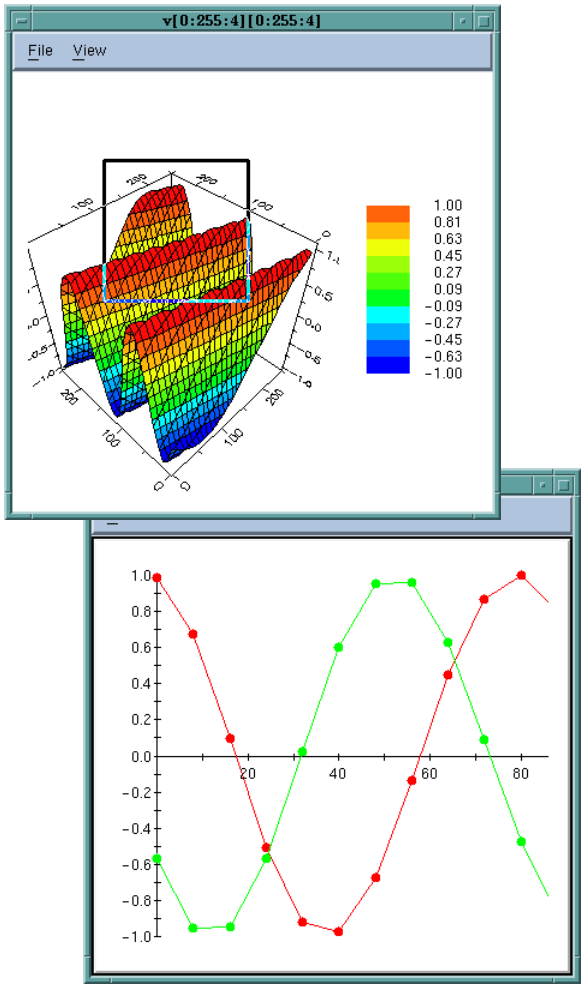
TotalView: Tools Menu

- Call Graph



- Message queue graph

- Data visualization



MUST

- Next generation MPI correctness and portability checker
- http://doc.itc.rwth-aachen.de/display/CCP/Project+MUST

- MUST reports
  - Errors: violations of the MPI-standard
  - Warnings: unusual behavior or possible problems
  - Notes: harmless but remarkable behavior
  - Further: potential deadlock detection
- Usage
  - Relink application with mustc, mustcxx, mustf90, …
  - Run application under the control of mustrun (requires one additional MPI process)
  - See MUST_Output.html report

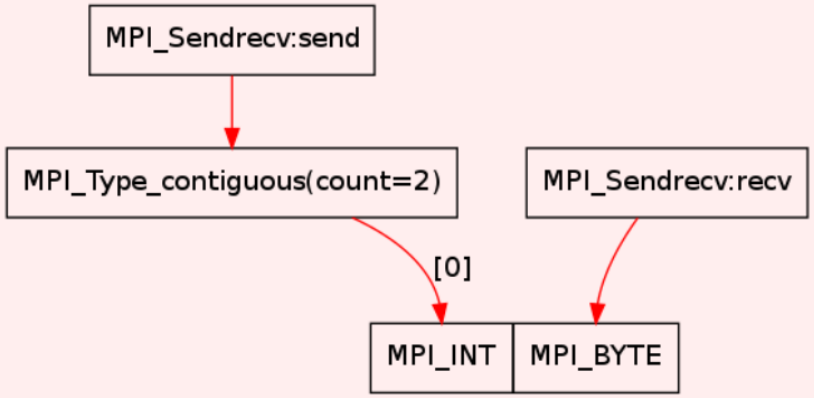
MUST Datatype Mismatch

Rank	Type	Message	From	References
0	Error	A send and a receive operation use datatypes that do not match! Mismatch occurs at (contiguous) [0](MPI_INT) in the send type and at (MPI_BYTE) in the receive type (consult the MUST manual for a detailed description of datatype positions). A graphical representation of this situation is available in a detailed type mismatch view (MUST_Output-files/MUST_Typemismatch_0.html). The send operation was started at reference 1, the receive operation was started at reference 2. (Information on communicator: MPI_COMM_WORLD) (Information on send of count 1 with type:Datatype created at reference 3 is for C, commited at reference 4, based on the following type(s): { MPI_INT}Typemap = {(MPI_INT, 0), (MPI_INT, 4)}) (Information on receive of count 8 with type:MPI_BYTE)	**MPI_Sendrecv** called from: #0 main@example.c:33	reference 1 rank 0: **MPI_Sendrecv** called from: #0 main@example.c:33 reference 2 rank 1: **MPI_Sendrecv** called from: #0 main@example.c:33 reference 3 rank 0: **MPI_Type_contiguous** called from: #0 main@example.c:29 reference 4 rank 0: **MPI_Type_commit** called from: #0 main@example.c:30

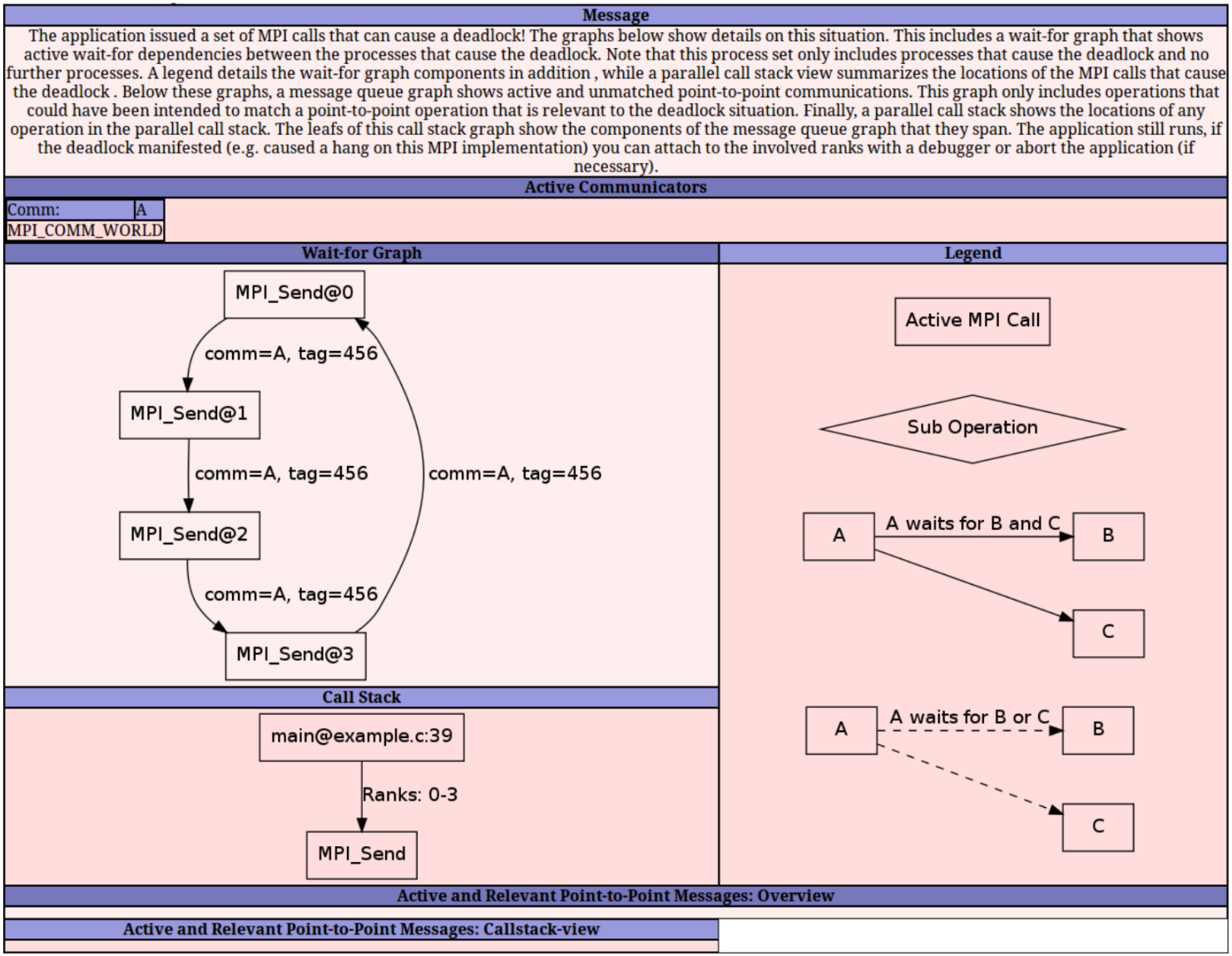
Message

The application issued a set of MPI calls that mismatch in type signatures! The graph below shows details on this situation. The first differing item of each involved communication request is highlighted.

Datatype Graph



MUST Deadlock Detection


Message
The application issued a set of MPI calls that can cause a deadlock! The graphs below show details on this situation. This includes a wait-for graph that shows active wait-for dependencies between the processes that cause the deadlock. Note that this process set only includes processes that cause the deadlock and no further processes. A legend details the wait-for graph components in addition , while a parallel call stack view summarizes the locations of the MPI calls that cause the deadlock . Below these graphs, a message queue graph shows active and unmatched point-to-point communications. This graph only includes operations that could have been intended to match a point-to-point operation that is relevant to the deadlock situation. Finally, a parallel call stack shows the locations of any operation in the parallel call stack. The leafs of this call stack graph show the components of the message queue graph that they span. The application still runs, if the deadlock manifested (e.g. caused a hang on this MPI implementation) you can attach to the involved ranks with a debugger or abort the application (if necessary).
Active Communicators
Comm: MPI_COMM_WORLD
A
Wait-for Graph
MPI_Send@0
comm=A, tag=456
MPI_Send@1
comm=A, tag=456
MPI_Send@2
comm=A, tag=456
MPI_Send@3
comm=A, tag=456
Legend
Active MPI Call
Sub Operation
A
A waits for B and C
B
C
A
A waits for B or C
B
C
Call Stack
main@example.c:39
Ranks: 0-3
MPI_Send
Active and Relevant Point-to-Point Messages: Overview
Active and Relevant Point-to-Point Messages: Callstack-view

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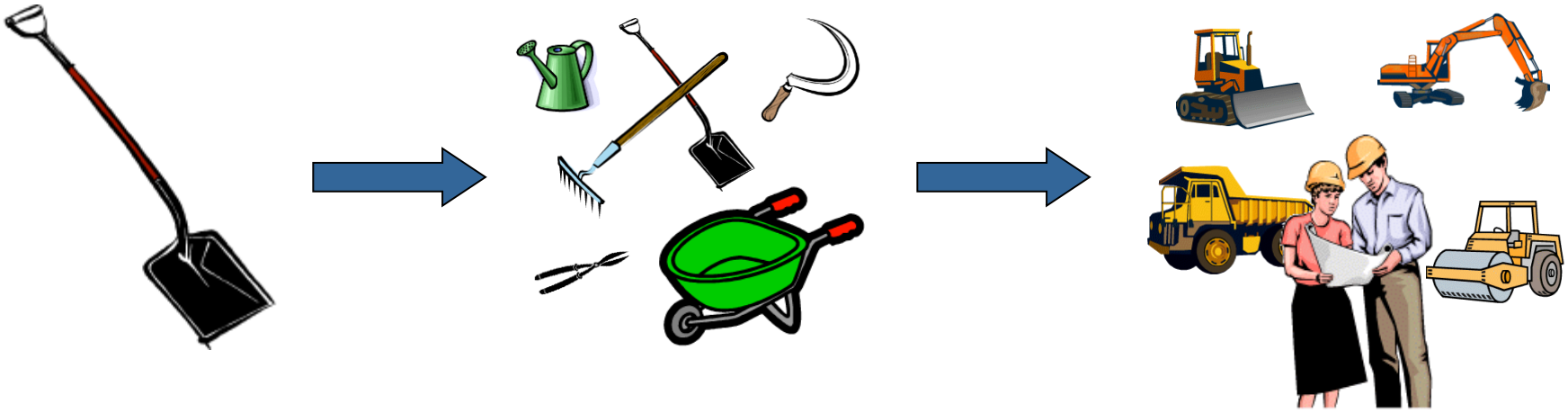
Performance Analysis Tools

Typical Performance Analysis Procedure

- Do I have a performance problem at all?
  - Time / speedup / scalability measurements
- ***What*** is the key bottleneck (computation / communication)?
  - MPI / OpenMP / flat profiling
- ***Where*** is the key bottleneck?
  - Call-path profiling, detailed basic block profiling
- ***Why*** is it there?
  - Hardware counter analysis
  - Trace selected parts (to keep trace size manageable)
- Does the code have scalability problems?
  - Load imbalance analysis, compare profiles at various sizes function-by-function

Remark: No Single Solution is Sufficient!



☞ *A combination of different methods, tools and techniques is typically needed!*

- Analysis
  - Statistics, visualization, automatic analysis, data mining, ...
- Measurement
  - Sampling / instrumentation, profiling / tracing, ...
- Instrumentation
  - Source code / binary, manual / automatic, ...

Critical Issues

- Accuracy
  - Intrusion overhead
    - Measurement itself needs time and thus lowers performance
  - Perturbation
    - Measurement alters program behavior, e.g., memory access pattern
    - Might prevent compiler optimization, e.g. function inlining
  - Accuracy of timers & counters
- Granularity
  - How many measurements?
  - How much information / processing during each measurement?

☞ *Tradeoff: Accuracy vs. Expressiveness of data*

Performance Tools (status: May 2015)

	JUQUEEN	JUROPATEST
Performance Tools		
Score-P measurement system	✓	✓
Scalasca2 performance analyzer	✓	✓
Vampir[Server] trace visualizer	✓	✓
HPCToolkit sampling profiler	✓	(✗)
Allinea Performance Reports	✗	✓
TAU performance system	✓	✓
mpiP MPI profiling library*	✓	✓
Extrae/Paraver tracing tool*	✓	✓
PAPI hardware counter library*	✓	✓

Score-P

- Community instrumentation and measurement infrastructure
  - Developed by a consortium of performance tool groups

  - Next generation measurement system of
    - Scalasca 2.x
    - Vampir
    - TAU
    - Periscope
- Common data formats improve tool interoperability
- http://www.score-p.org

scalasca

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German Research School for Simulation Sciences

- Collection of trace-based performance analysis tools
  - Specifically designed for large-scale systems
  - Unique features:
    - Scalable, automated search for event patterns representing inefficient behavior
    - Scalable identification of the critical execution path
    - Delay / root-cause analysis
- Based on Score-P for instrumentation and measurement
  - Includes convenience / post-processing commands providing added value
- http://www.scalasca.org

What is the Key Bottleneck?

- Generate flat MPI profile using Score-P/Scalasca (or mpiP)
  - Only requires re-linking
  - Low runtime overhead

- Provides detailed information on MPI usage
  - How much time is spent in which operation?
  - How often is each operation called?
  - How much data was transferred?

- Limitations:
  - Computation on non-master threads and outside of MPI_Init/MPI_Finalize scope ignored

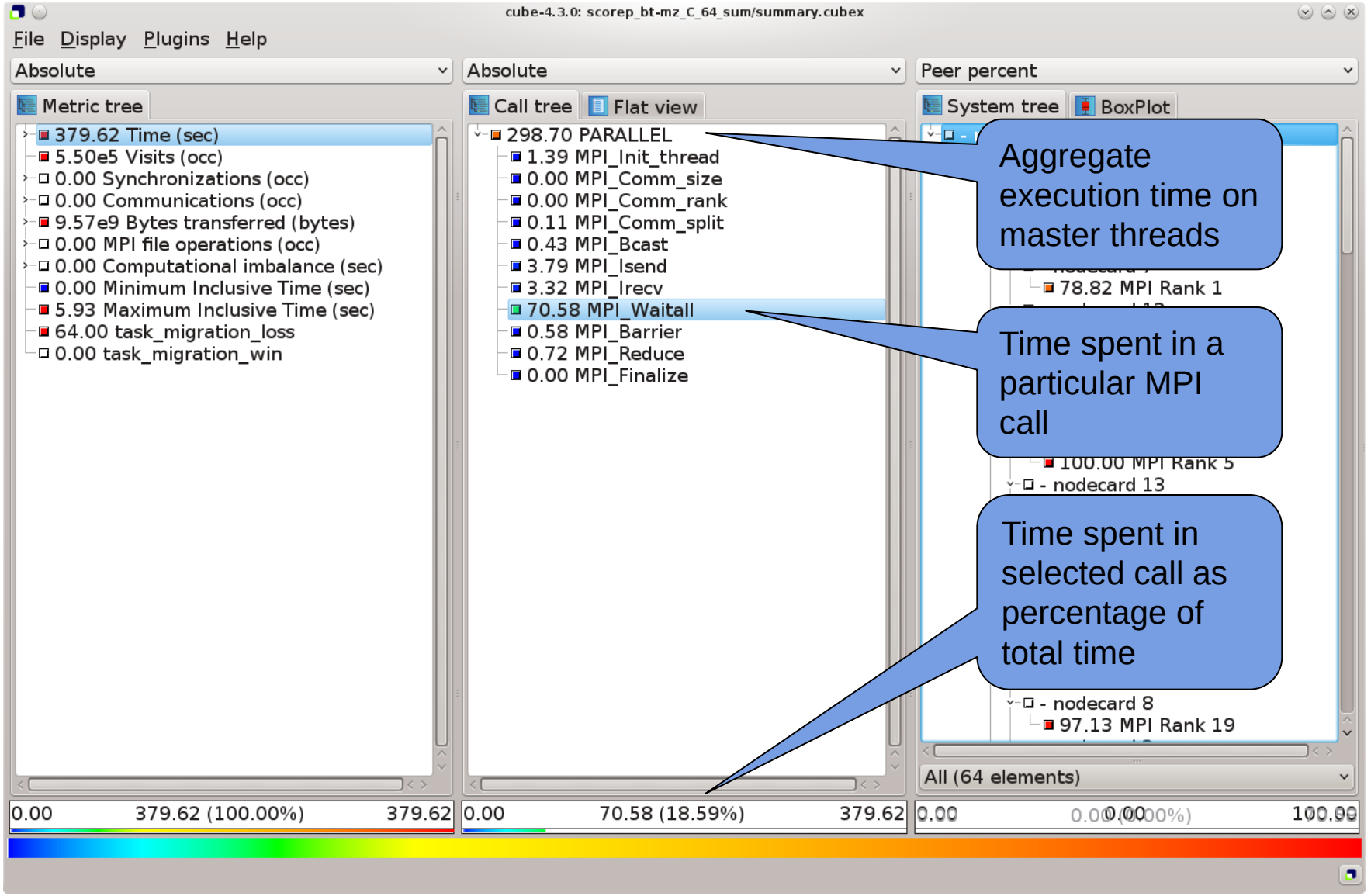
Flat MPI Profile: Recipe

1. Prefix your ***link command*** with
   "`scorep --nocompiler`"
2. Prefix your MPI ***launch command*** with
   "`scalasca -analyze`"
3. After execution, examine analysis results using
   "`scalasca -examine scorep_<title>`"

Flat MPI Profile: Example

```
% module load UNITE scorep scalasca
% mpixlf90 -O3 -qsmp=omp -c foo.f90
% mpixlf90 -O3 -qsmp=omp -c bar.f90
% scorep --nocompiler \
    mpixlf90 -O3 -qsmp=omp -o myprog foo.o bar.o

############################
##  In the job script:  ##
############################

module load UNITE scalasca
scalasca -analyze \
    runjob --ranks-per-node P --np n [...] --exe ./myprog

############################
## After job finished:  ##
############################

% scalasca -examine scorep_myprog_Ppnxt_sum
```

Flat MPI Profile: Example (cont.)



Where is the Key Bottleneck?

- Generate call-path profile using Score-P/Scalasca
  - Requires re-compilation
  - Runtime overhead depends on application characteristics
  - Typically needs some care setting up a good measurement configuration
    - Filtering
    - Selective instrumentation

- Option 1 (recommended):
  Automatic compiler-based instrumentation

- Option 2:
  Manual instrumentation of interesting phases, routines, loops

Call-path Profile: Recipe

1. Prefix your ***compile & link commands*** with
   "`scorep`"
2. Prefix your MPI ***launch command*** with
   "`scalasca -analyze`"
3. After execution, compare overall runtime with uninstrumented run to determine overhead
4. If overhead is too high
   1. Score measurement using
      "`scalasca -examine -s scorep_<title>`"
   2. Prepare filter file
   3. Re-run measurement with filter applied using prefix
      "`scalasca -analyze -f <filter_file>`"
5. After execution, examine analysis results using
   "`scalasca -examine scorep_<title>`"

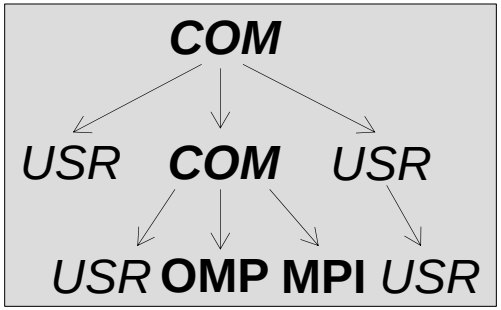
Call-path Profile: Example

```
% module load UNITE scorep scalasca
% scorep mpixlf90 -O3 -qsmp=omp -c foo.f90
% scorep mpixlf90 -O3 -qsmp=omp -c bar.f90
% scorep \
    mpixlf90 -O3 -qsmp=omp -o myprog foo.o bar.o



############################
##  In the job script:  ##
############################

module load UNITE scalasca
scalasca -analyze \
    runjob --ranks-per-node P --np n [...] --exe ./myprog
```

Call-path Profile: Example (cont.)

```
% scalasca -examine -s epik_myprog_Ppnxt_sum
scorep-score -r ./epik_myprog_Ppnxt_sum/profile.cubex
INFO: Score report written to ./scorep_myprog_Ppnxt_sum/scorep.score
```

- Estimates trace buffer requirements
- Allows to identify canditate functions for filtering
  - ☞ Computational routines with high visit count and low time-per-visit ratio
- Region/call-path classification
  - MPI (pure MPI library functions)
  - OMP (pure OpenMP functions/regions)
  - USR (user-level source local computation
  - COM (“combined” USR + OpeMP/MPI)
  - ANY/ALL (aggregate of all region types)



Call-path Profile: Example (cont.)

```
% less scorep_myprog_Ppmxt_sum/scorep.score
Estimated aggregate size of event trace:                   162GB
Estimated requirements for largest trace buffer (max_buf): 2758MB
Estimated memory requirements (SCOREP_TOTAL_MEMORY):       2822MB
(hint: When tracing set SCOREP_TOTAL_MEMORY=2822MB to avoid
 intermediate flushes or reduce requirements using USR regions
 filters.)

flt type    max_buf[B]         visits  time[s] time[%] time/     region
                                                       visit[us]
     ALL 2,891,417,902 6,662,521,083 36581.51   100.0      5.49  ALL
     USR 2,858,189,854 6,574,882,113 13618.14    37.2      2.07  USR
     OMP    54,327,600    86,353,920 22719.78    62.1    263.10  OMP
     MPI       676,342       550,010   208.98     0.6    379.96  MPI
     COM       371,930       735,040    34.61     0.1     47.09  COM

     USR   921,918,660 2,110,313,472  3290.11     9.0      1.56  matmul_sub
     USR   921,918,660 2,110,313,472  5914.98    16.2      2.80  binvcrhs
     USR   921,918,660 2,110,313,472  3822.64    10.4      1.81  matvec_sub
     USR    41,071,134    87,475,200   358.56     1.0      4.10  lhsinit
     USR    41,071,134    87,475,200   145.42     0.4      1.66  binvrhs
     USR    29,194,256    68,892,672    86.15     0.2      1.25  exact_solution
     OMP     3,280,320     3,293,184    15.81     0.0      4.80  !$omp parallel
     [...]
```

Call-path Profile: Filtering

- In this example, the 6 most fequently called routines are of type USR
- These routines contribute around 35% of total time
  - However, much of that is most likely measurement overhead
    - Frequently executed
    - Time-per-visit ratio in the order of a few microseconds

☞ Avoid measurements to reduce the overhead

☞ List routines to be filtered in simple text file

Filtering: Example

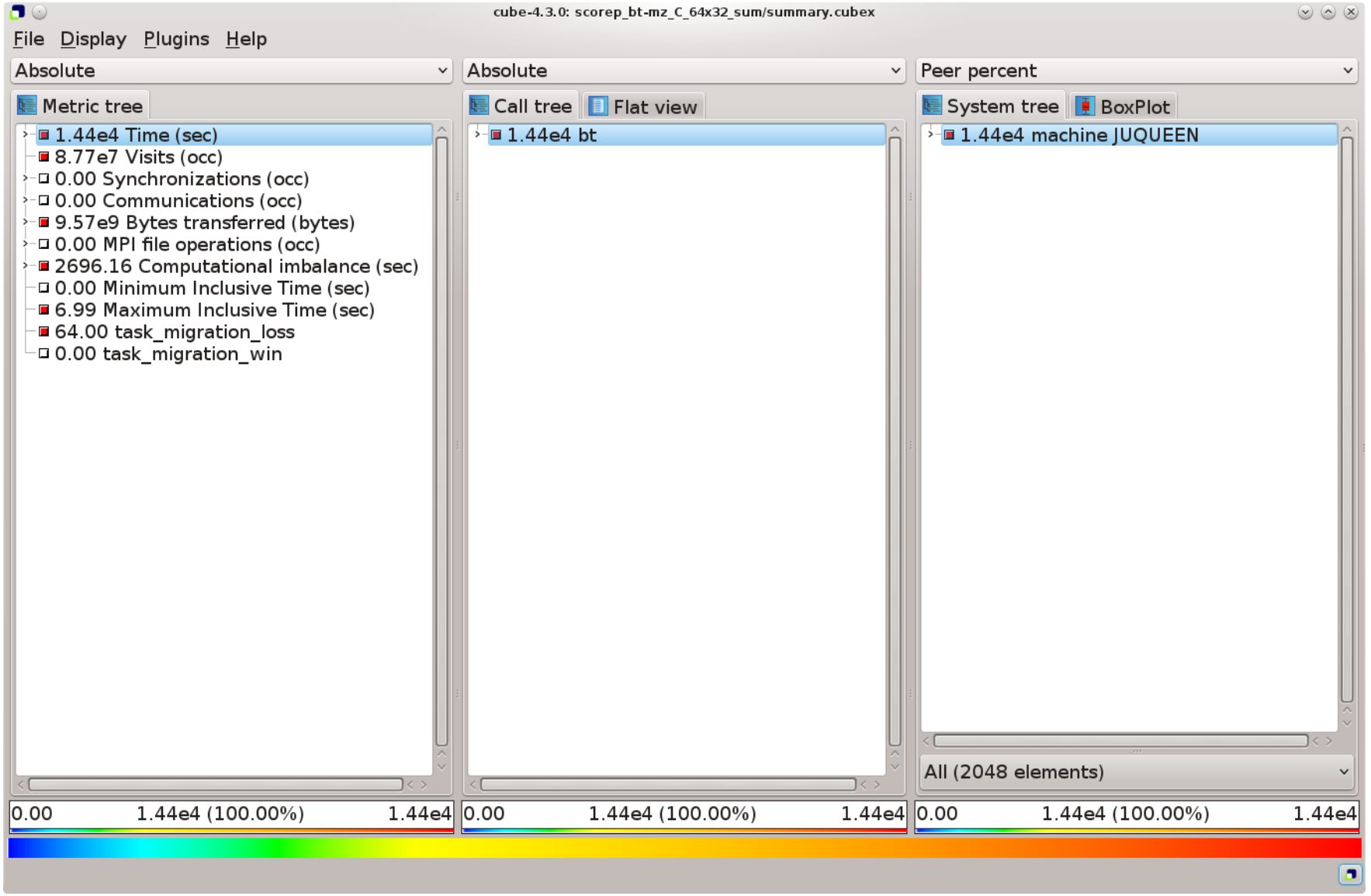
```
% cat filter.txt
SCOREP_REGION_NAMES_BEGIN
    EXCLUDE
        binvcrhs
        matmul_sub
        matvec_sub
        binvrhs
        lhsinit
        exact_solution
SCOREP_REGION_NAMES_END
```

- Score-P filtering files support
  - Wildcards (shell globs)
  - Blacklisting
  - Whitelisting
  - Filtering based on filenames

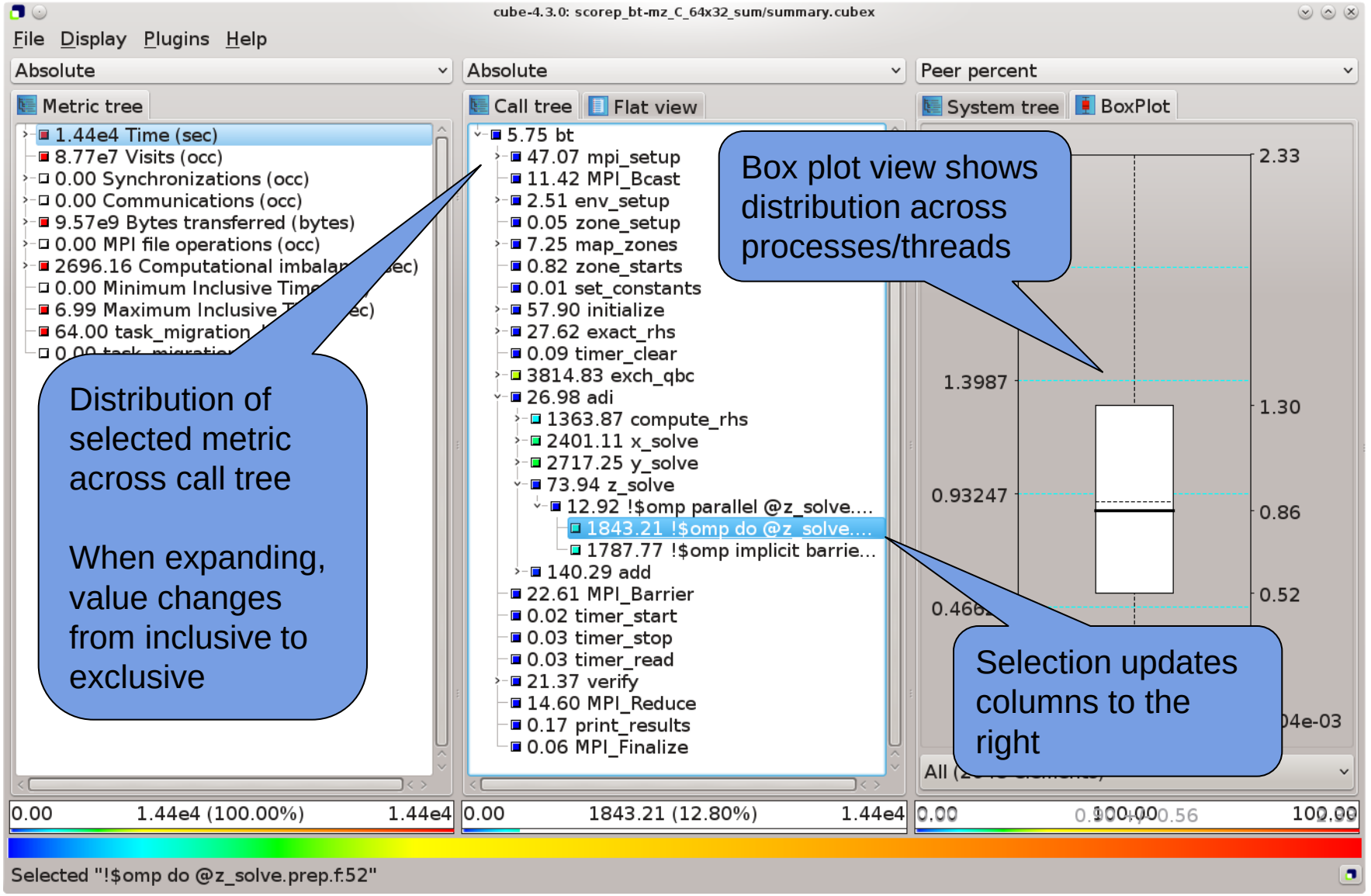
Call-path Profile: Example (cont.)

```
##  To verify effect of filter:

% scalasca -examine -s -f filter.txt \
    scorep_myprog_Ppnxt_sum

############################
##  In the job script:  ##
############################

module load UNITE scalasca
scalasca -analyze -f filter.txt \
    runjob --ranks-per-node P --np n [...] --exe ./myprog

############################
## After job finished:  ##
############################

% scalasca -examine scorep_myprog_Ppnxt_sum
```

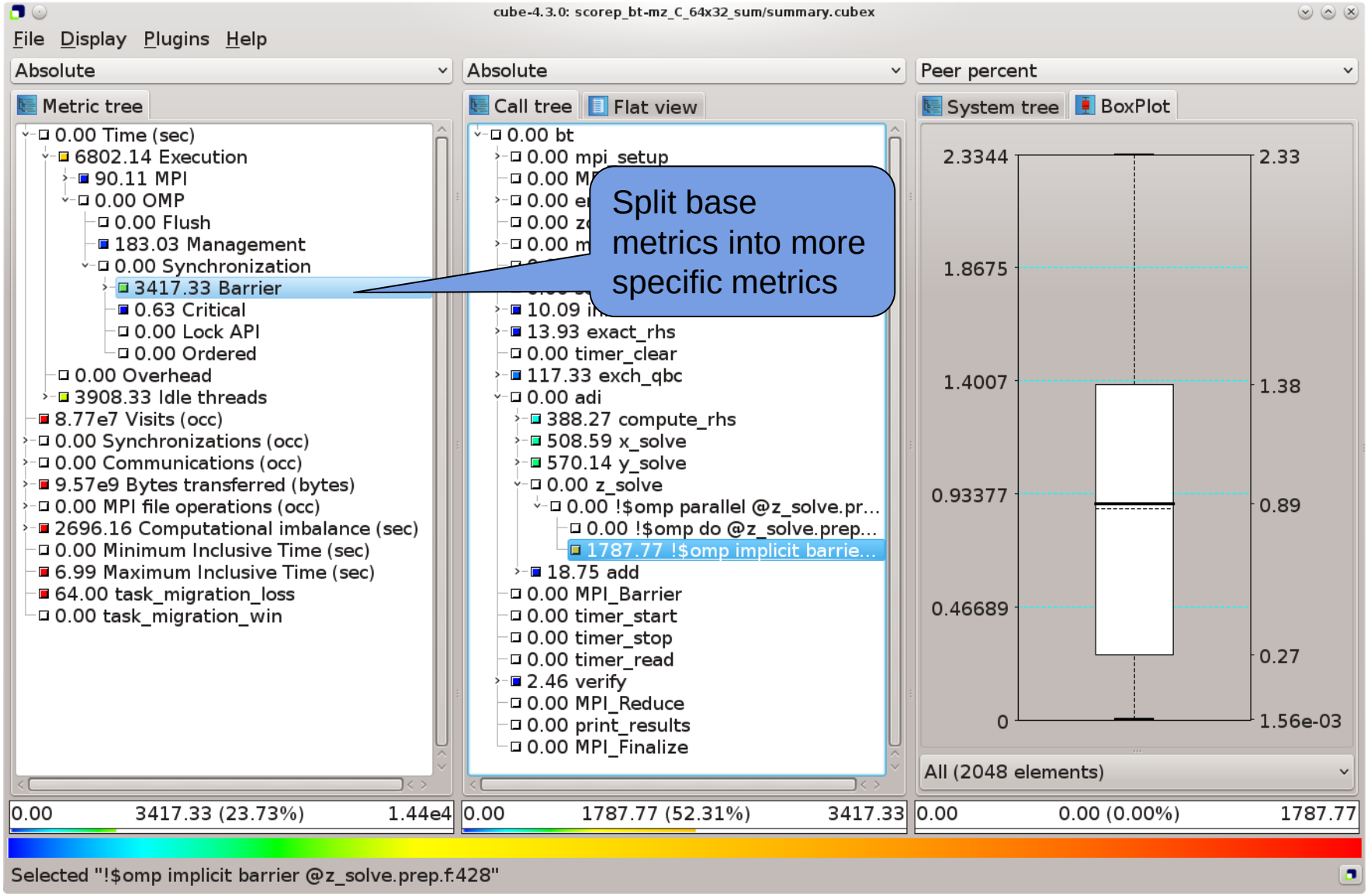
Call-path Profile: Example (cont.)



Call-path Profile: Example (cont.)



Call-path Profile: Example (cont.)



Score-P: Advanced Features

- Measurement can be extensively configured via environment variables
  - Check output of "`scorep-info config-vars`" for details
- Allows for targeted measurements:
  - Selective recording
  - Phase profiling
  - Parameter-based profiling
  - …
- Please ask us or see the user manual for details

Why is the Bottleneck There?

- This is highly application dependent!
- Might require additional measurements
  - Hardware-counter analysis
    - CPU utilization
    - Cache behavior
  - Selective instrumentation
  - Manual/automatic event trace analysis

HW Counter Measurements w/ Score-P

- Score-P supports both PAPI preset and native counters
- Available counters: `papi_avail` or `papi_native_avail`

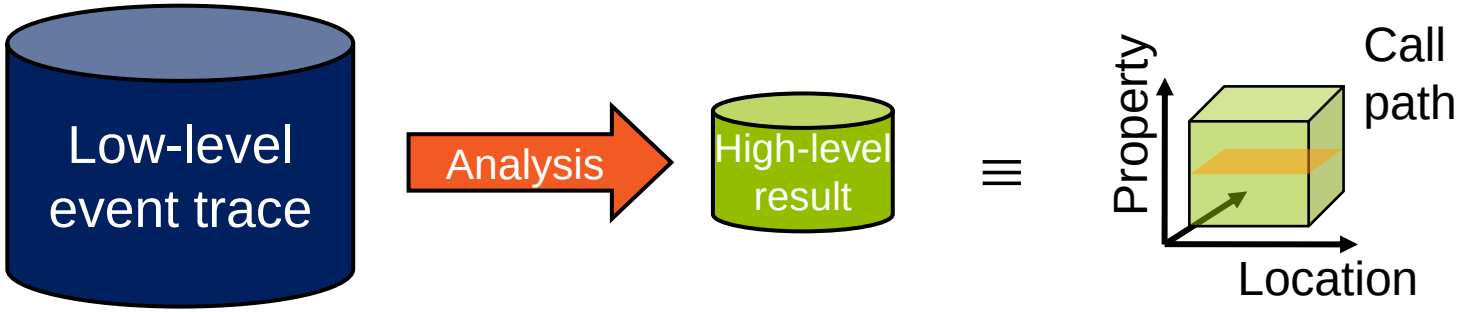
```
% module load UNITE papi/5.0.1
% less $PAPI_ROOT/doc/papi-5.0.1-avail.txt
% less $PAPI_ROOT/doc/papi-5.0.1-native_avail.txt
% less $PAPI_ROOT/doc/papi-5.0.1-avail-detail.txt
```

- Specify using “SCOREP_METRIC_PAPI” environment variable

```
############################
##  In the job script:  ##
############################

module load UNITE scalasca
export SCOREP_METRIC_PAPI=“PAPI_FP_OPS,PAPI_TOT_CYC“
scalasca -analyze -f filter.txt \
runjob --ranks-per-node P --np n [...] --exe ./myprog
```

Automatic Trace Analysis w/ Scalasca

- Idea: Automatic search for patterns of inefficient behavior
  - Identification of wait states and their root causes
  - Classification of behavior & quantification of significance
  - Scalable identification of the critical execution path



- Advantages
  - Guaranteed to cover the entire event trace
  - Quicker than manual/visual trace analysis
  - Helps to identify hot-spots for in-depth manual analysis

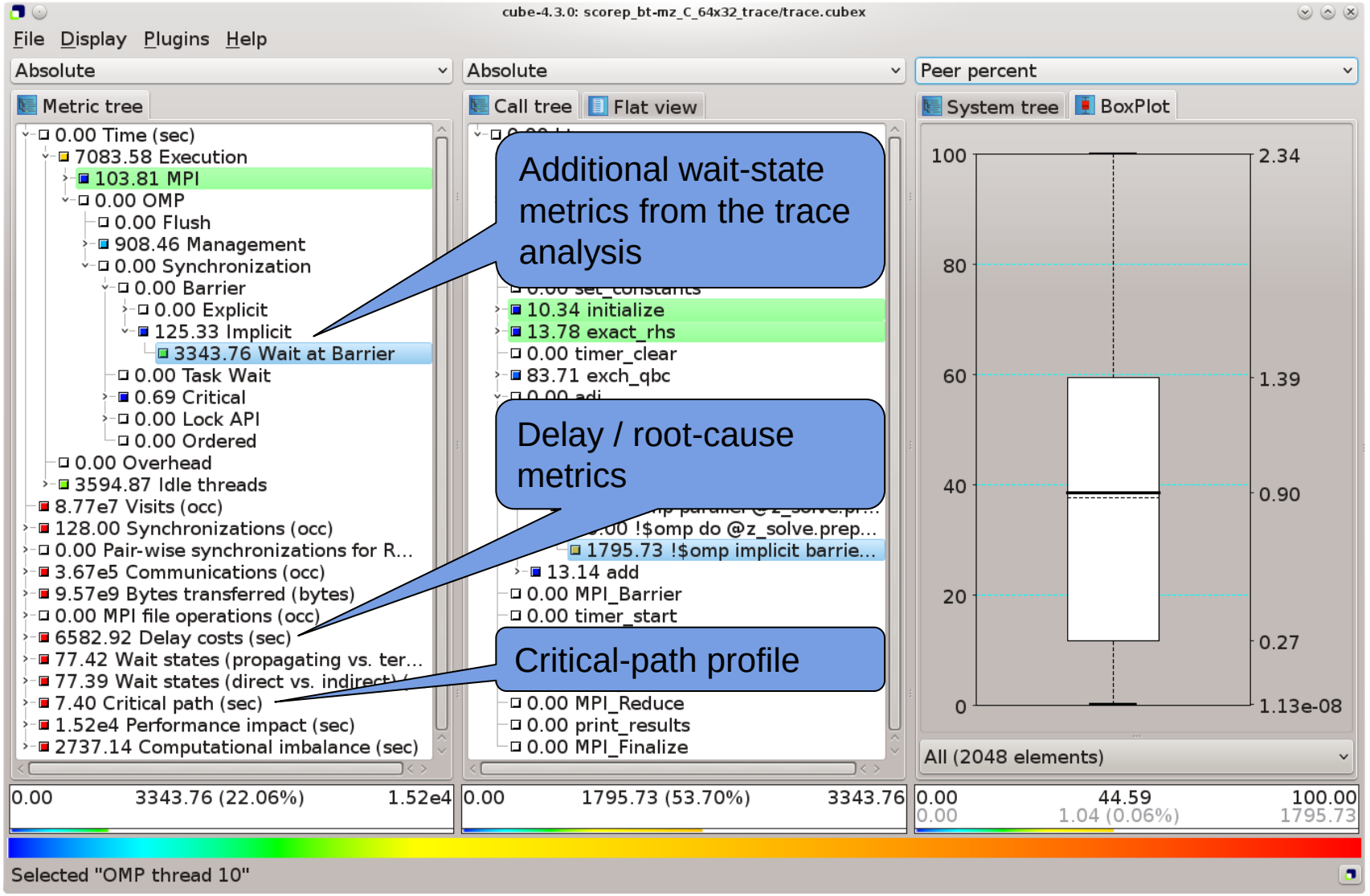
Trace Generation & Analysis w/ Scalasca

- Enable trace collection & analysis using "`-t`" option of "`scalasca -analyze`":

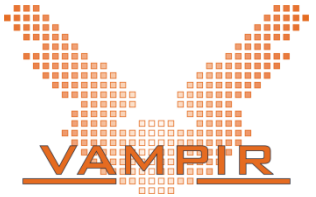
```
############################
##  In the job script:  ##
############################

module load UNITE scalasca
export SCOREP_TOTAL_MEMORY=120MB   # Consult score report
scalasca -analyze -f filter.txt -t \
    runjob --ranks-per-node P --np n [...] --exe ./myprog
```

- **ATTENTION:**
  - Traces can quickly become extremely large!
  - Remember to use proper filtering, selective instrumentation, and Score-P memory specification
  - Before flooding the file system, **ask us for assistance!**

Scalasca Trace Analysis Example



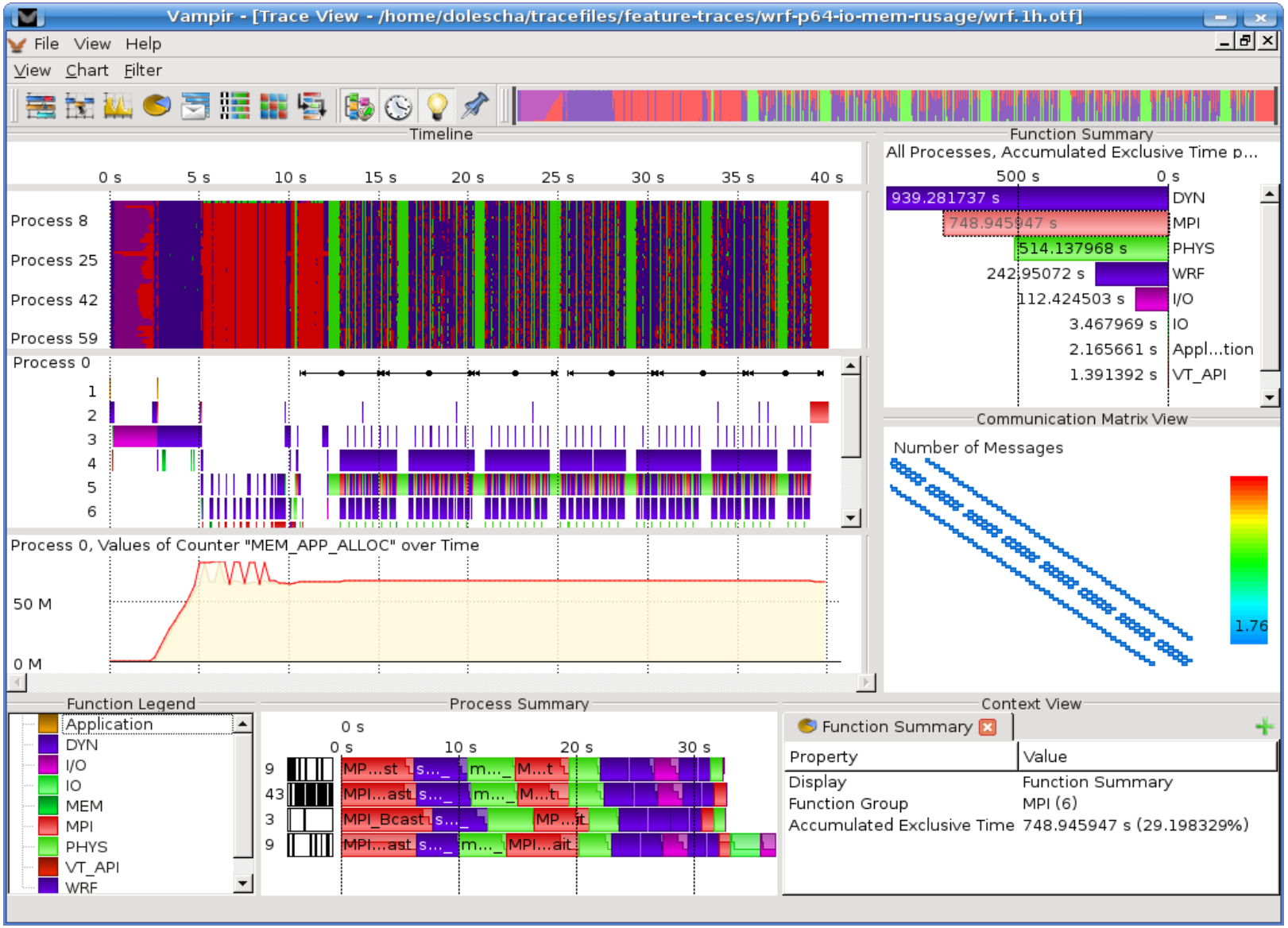
Vampir Event Trace Visualizer



- Offline trace visualization for Score-P's OTF2 trace files
- Visualization of MPI, OpenMP and application events:
  - All diagrams highly customizable (through context menus)
  - Large variety of displays for ANY part of the trace
- http://www.vampir.eu

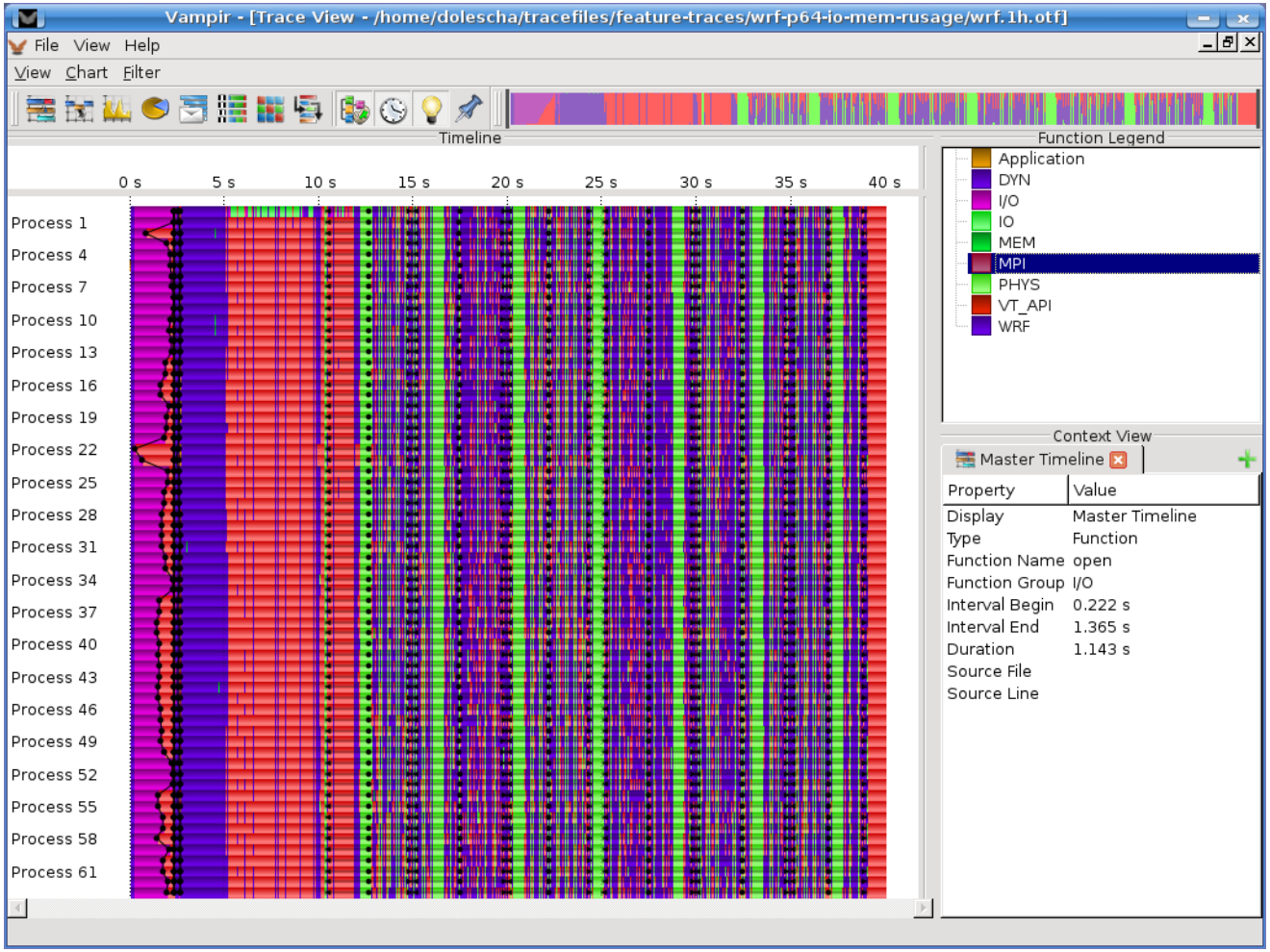
- Advantage:
  - Detailed view of dynamic application behavior
- Disadvantage:
  - Requires event traces (huge amount of data)
  - Completely manual analysis

Vampir Displays



Vampir: Timeline Diagram

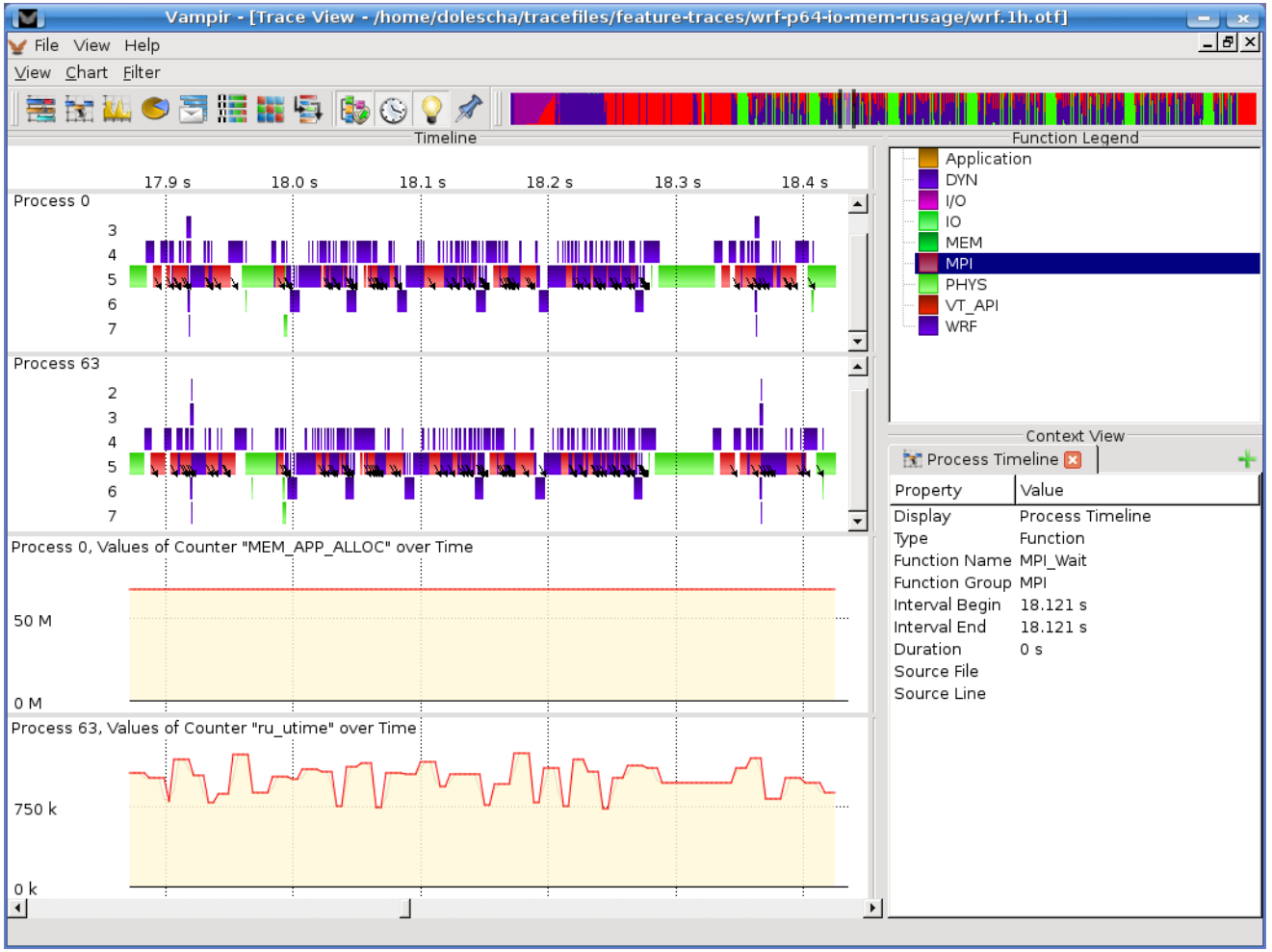
- Functions organized into groups
- coloring by group
- Message lines can be colored by tag or size



- Information about states, messages, collective and I/O operations available through clicking on the representation

Vampir: Process and Counter Timelines

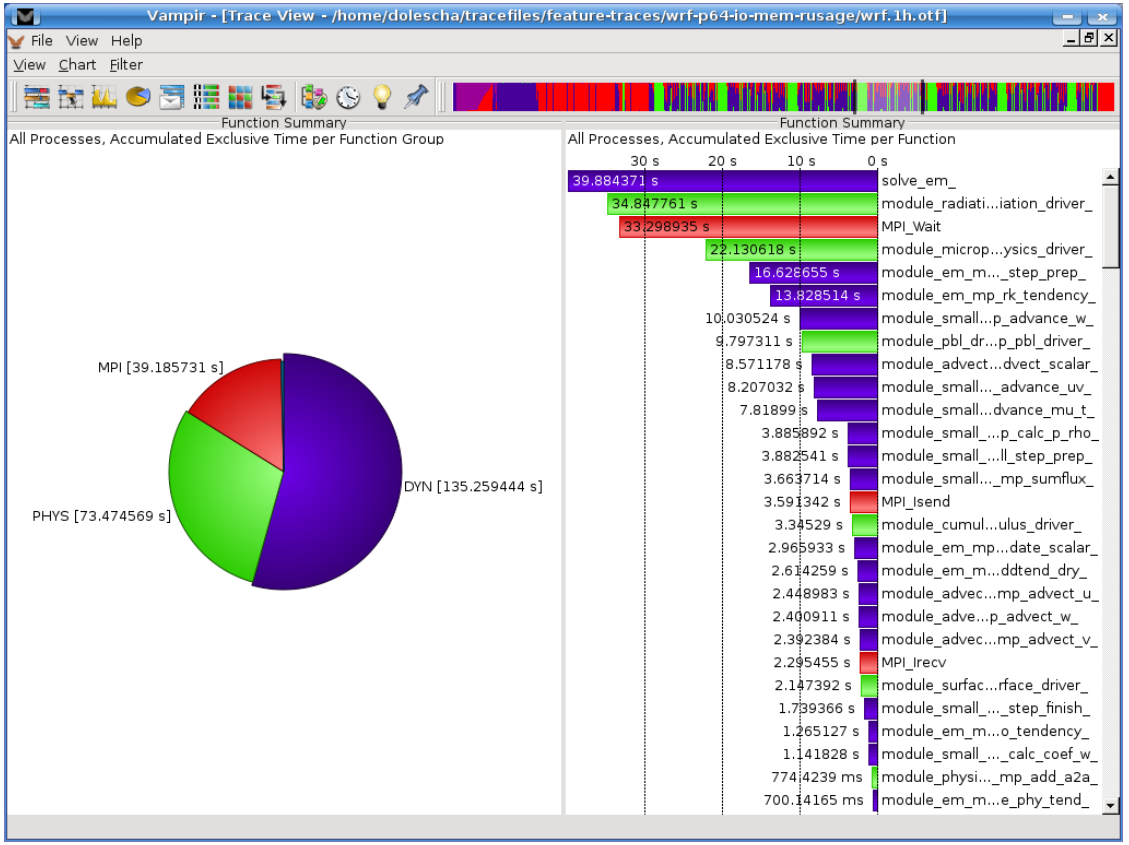
- Process timeline show call stack nesting
- Counter timelines for hardware or software counters



Vampir: Execution Statistics

- Aggregated profiling information: execution time, number of calls, inclusive/exclusive

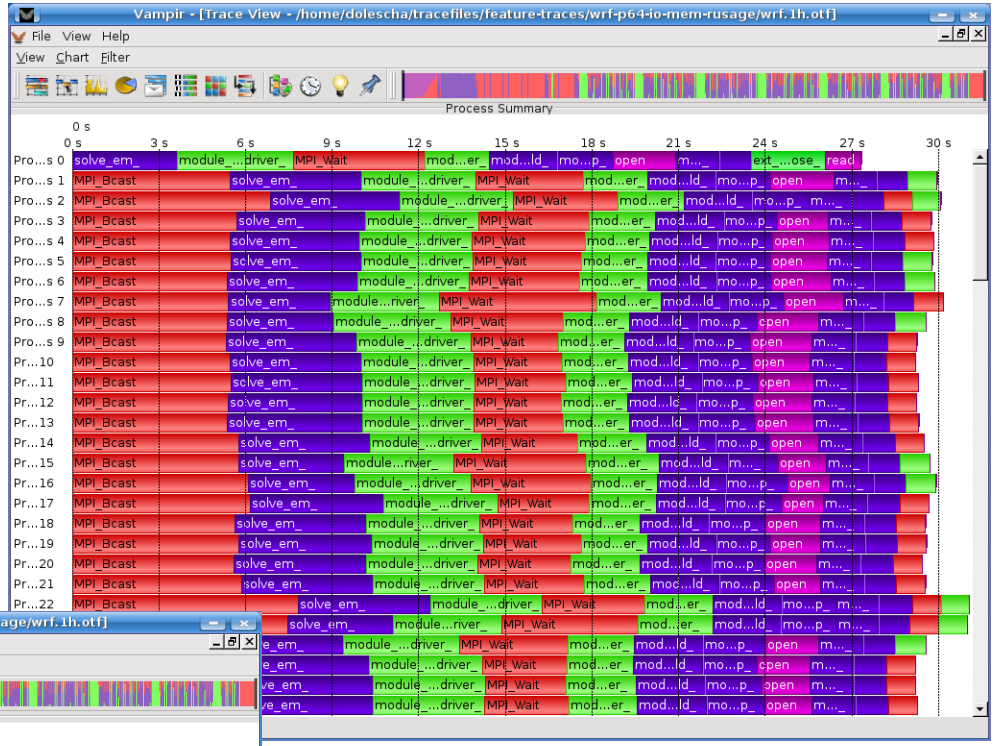
- Available for all / any group (activity) or all routines (symbols)

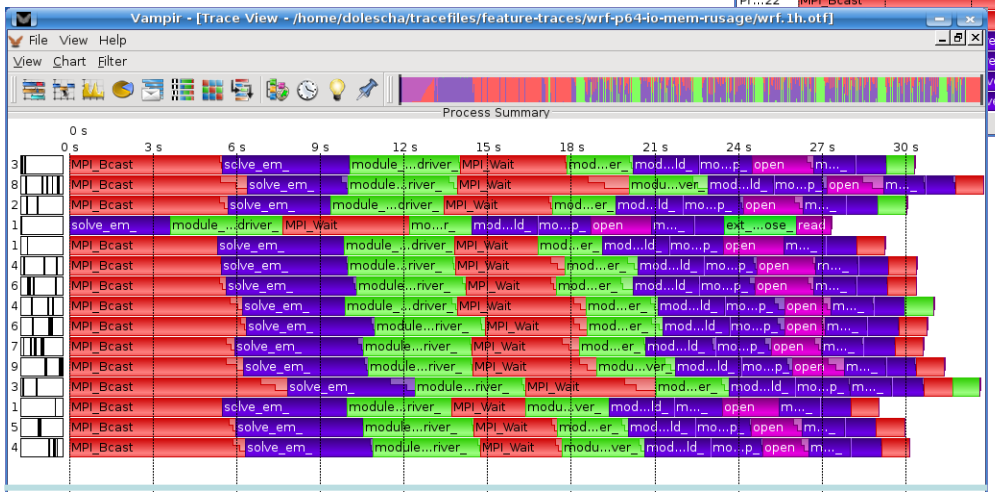


- Available for any part of the trace
  ⇨ selectable through time line diagram

Vampir: Process Summary

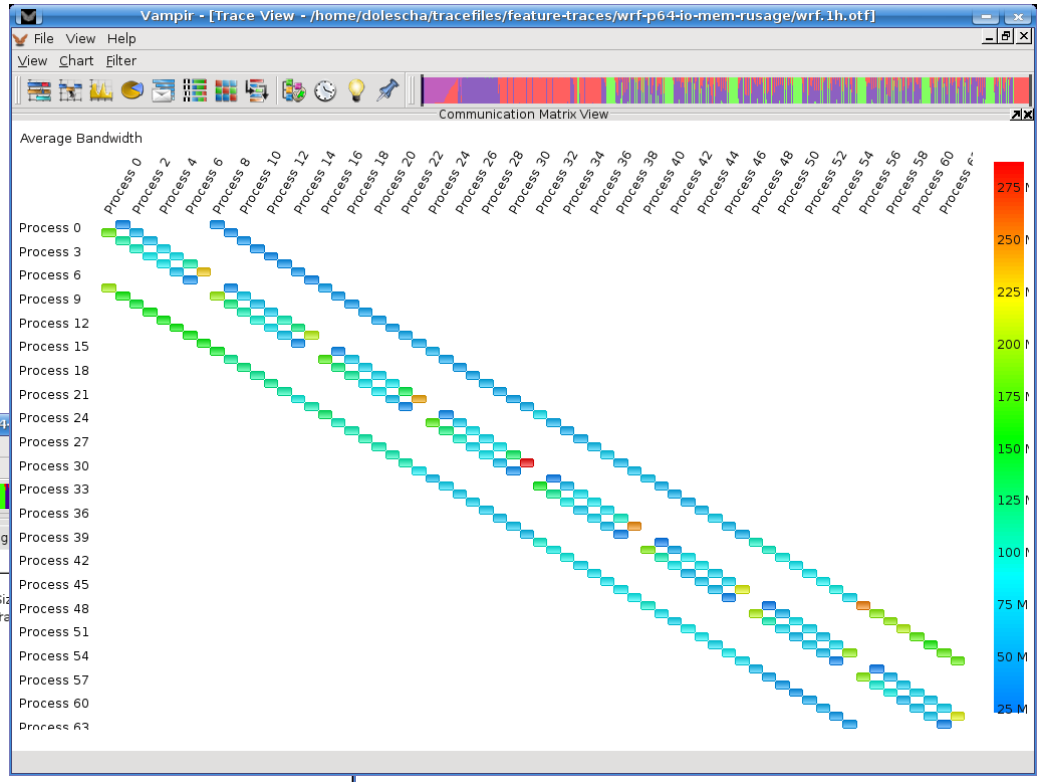
- Execution statistics over all processes for comparison
- Clustering mode available for large process counts

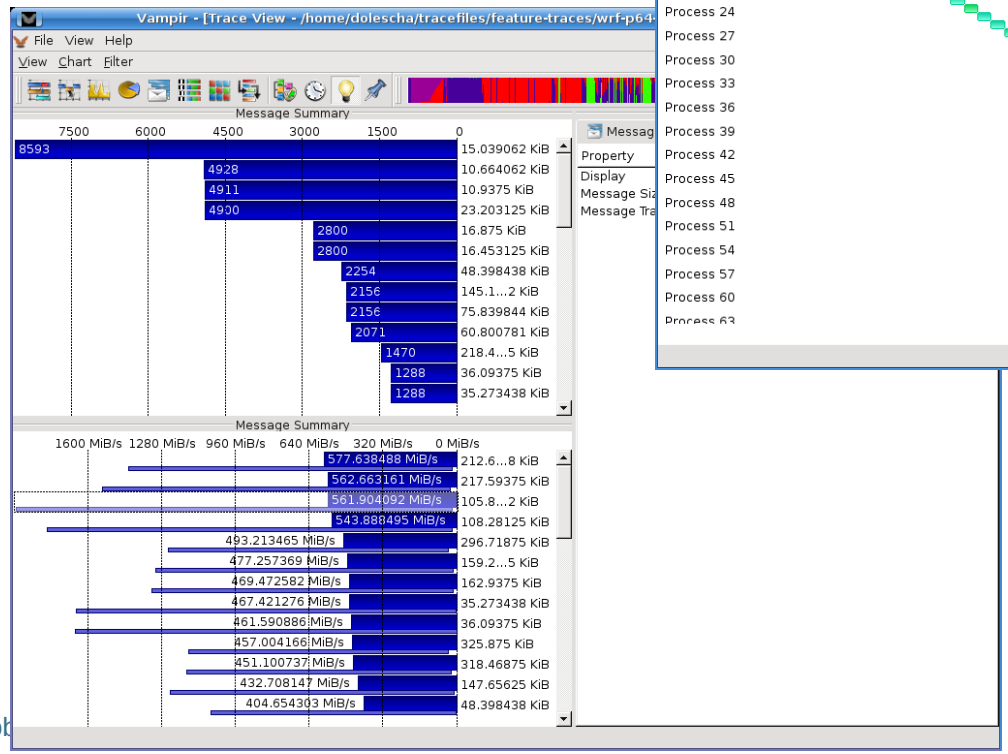




Vampir: Communication Statistics

- Byte and message count, min/max/avg message length and min/max/avg bandwidth for each process pair
- Message length statistics





- Available for any part of the trace

HPCToolkit (Rice University)

JÜLICH FORSCHUNGSZENTRUM

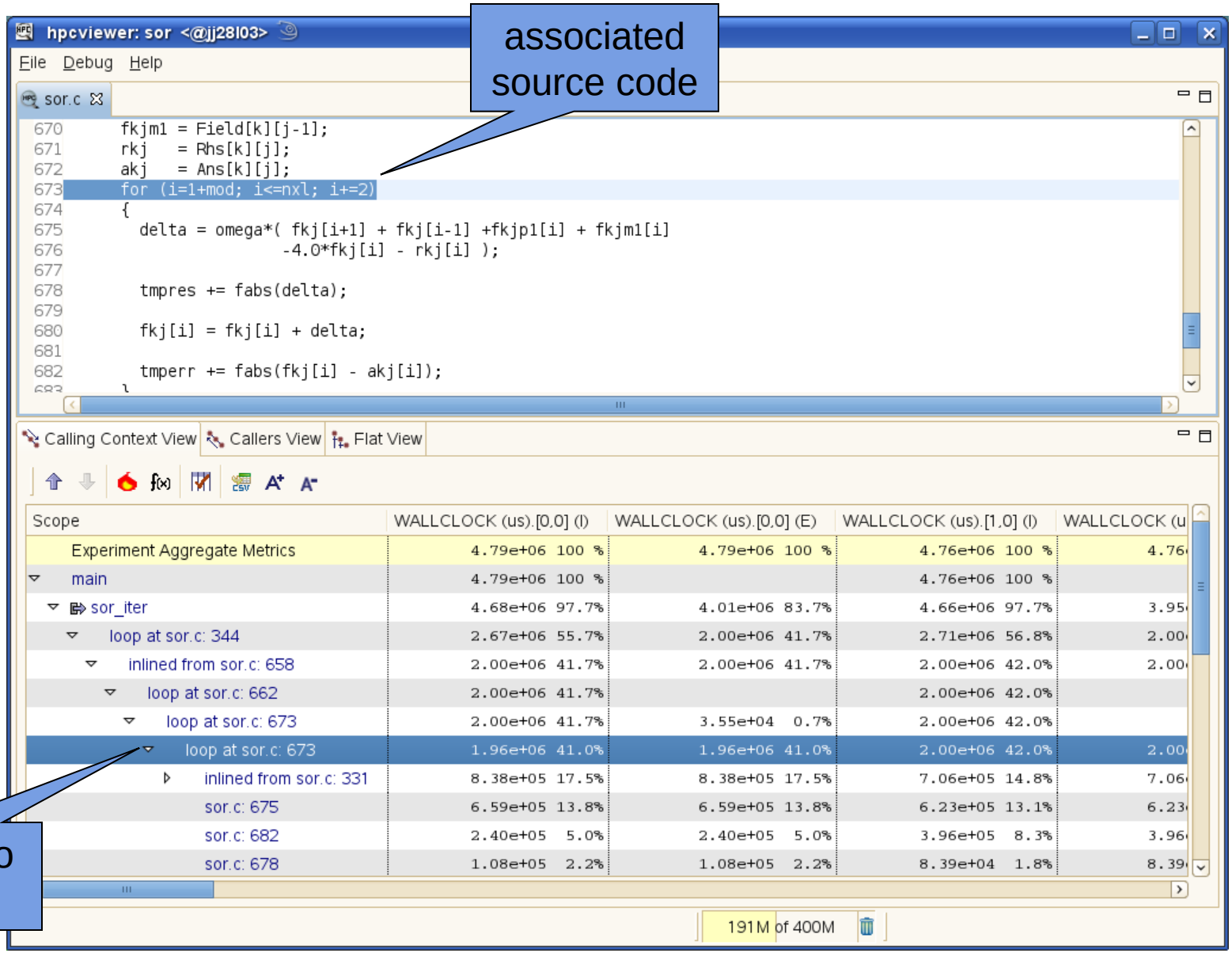
- Multi-platform sampling-based call-path profiler
- Works on unmodified, optimized executables
- http://hpctoolkit.org

- Advantages:
  - Overhead can be easily controlled via sampling interval
  - Advantageous for complex C++ codes with many small functions
  - Loop-level analysis (sometimes even individual source lines)
  - Supports POSIX threads
- Disadvantages:
  - Statistical approach that might miss details
  - MPI/OpenMP time displayed as low-level system calls

HPCToolkit: Metric Specification

- Specified via environment variable `HPCRUN_EVENT_LIST`
- General format:
  "`name@interval [;name@interval ...]`"
- Possible sample sources:
  - WALLCLOCK
  - PAPI counters
  - IO (use w/o interval spec)
  - MEMLEAK (use w/o interval spec)
- Interval: given in microseconds
  - E.g., 10000 → 100 samples per second

Example: hpcviewer


hpcviewer: sor <@jj28l03>
File Debug Help
sor.c
670 fkjm1 = Field[k][j-1];
671 rkj = Rhs[k][j];
672 akj = Ans[k][j];
673 for (i=1+mod; i<=nxl; i+=2)
674 {
675 delta = omega*(fkj[i+1] + fkj[i-1] +fkjp1[i] + fkjm1[i]
676 -4.0*fkj[i] - rkj[i]);
677
678 tmpres += fabs(delta);
679
680 fkj[i] = fkj[i] + delta;
681
682 tmperr += fabs(fkj[i] - akj[i]);
Calling Context View
Callers View
Flat View
Scope
WALLCLOCK (us).[0,0] (I)
WALLCLOCK (us).[0,0] (E)
WALLCLOCK (us).[1,0] (I)
Experiment Aggregate Metrics 4.79e+06 100 % 4.79e+06 100 % 4.76e+06 100 %
main 4.79e+06 100 % 4.76e+06 100 %
sor_iter 4.68e+06 97.7% 4.01e+06 83.7% 4.66e+06 97.7%
loop at sor.c: 344 2.67e+06 55.7% 2.00e+06 41.7% 2.71e+06 56.8%
inlined from sor.c: 658 2.00e+06 41.7% 2.00e+06 41.7% 2.00e+06 42.0%
loop at sor.c: 662 2.00e+06 41.7% 2.00e+06 42.0%
loop at sor.c: 673 2.00e+06 41.7% 3.55e+04 0.7% 2.00e+06 42.0%
loop at sor.c: 673 1.96e+06 41.0% 1.96e+06 41.0% 2.00e+06 42.0%
inlined from sor.c: 331 8.38e+05 17.5% 8.38e+05 17.5% 7.06e+05 14.8%
sor.c: 675 6.59e+05 13.8% 6.59e+05 13.8% 6.23e+05 13.1%
sor.c: 682 2.40e+05 5.0% 2.40e+05 5.0% 3.96e+05 8.3%
sor.c: 678 1.08e+05 2.2% 1.08e+05 2.2% 8.39e+04 1.8%
191M of 400M
associated source code
Callpath to hotspot

Allinea Performance Reports

- Single page report provides quick overview of performance issues
- Works on unmodified, optimized executables
- Shows CPU, memory, network and I/O utilization
- http://www.allinea.com/products/allinea-performance-reports

- Supports MPI, multi-threading and accelerators
- Saves data in HTML, CVS or text form

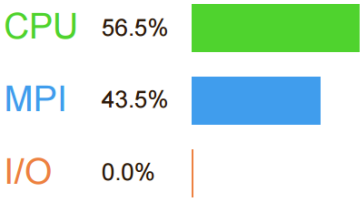
- Note: License limited to 512 processes (with unlimited number of threads)

Example Performance Reports

JÜLICH FORSCHUNGSZENTRUM

Summary: cp2k.popt is CPU-bound in this configuration

The total wallclock time was spent as follows:



Time spent running application code. High values are usually good.
This is **average**; check the CPU performance section for optimization advice.

Time spent in MPI calls. High values are usually bad.
This is **average**; check the MPI breakdown for advice on reducing it.

Time spent in filesystem I/O. High values are usually bad.
This is **negligible**; there's no need to investigate I/O performance.

This application run was CPU-bound. A breakdown of this time and advice for investigating further is in the CPU section below.

CPU

A breakdown of how the 56.5% total CPU time was spent:

Scalar numeric ops	27.7%
Vector numeric ops	11.3%
Memory accesses	60.9%
Other	0.0

The per-core performance is memory-bound. Use a profiler to identify time-consuming loops and check their cache performance.

Little time is spent in vectorized instructions. Check the compiler's vectorization advice to see why key loops could not be vectorized.

MPI

Of the 43.5% total time spent in MPI calls:

Time in collective calls	8.2%
Time in point-to-point calls	91.8%
Estimated collective rate	169 Mb/s
Estimated point-to-point rate	50.6 Mb/s

The point-to-point transfer rate is low. This can be caused by inefficient message sizes, such as many small messages, or by imbalanced workloads causing processes to wait. Use an MPI profiler to identify the problematic calls and ranks.

I/O

A breakdown of how the 0.0% total I/O time was spent:

Time in reads	0.0%
Time in writes	0.0%
Estimated read rate	0 bytes/s
Estimated write rate	0 bytes/s

No time is spent in I/O operations. There's nothing to optimize here!

Memory

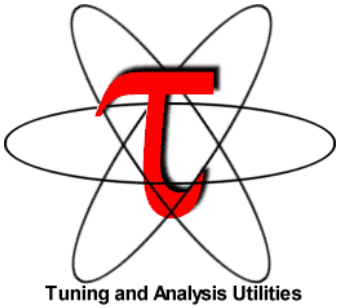
Per-process memory usage may also affect scaling:

Mean process memory usage	82.5 Mb
Peak process memory usage	89.3 Mb
Peak node memory usage	7.4%

The peak node memory usage is low. You may be able to reduce the total number of CPU hours used by running with fewer MPI processes and more data on each process.

TAU

- Very portable tool set for instrumentation, measurementand analysis of parallel multi-threaded applications
- http://tau.uoregon.edu/

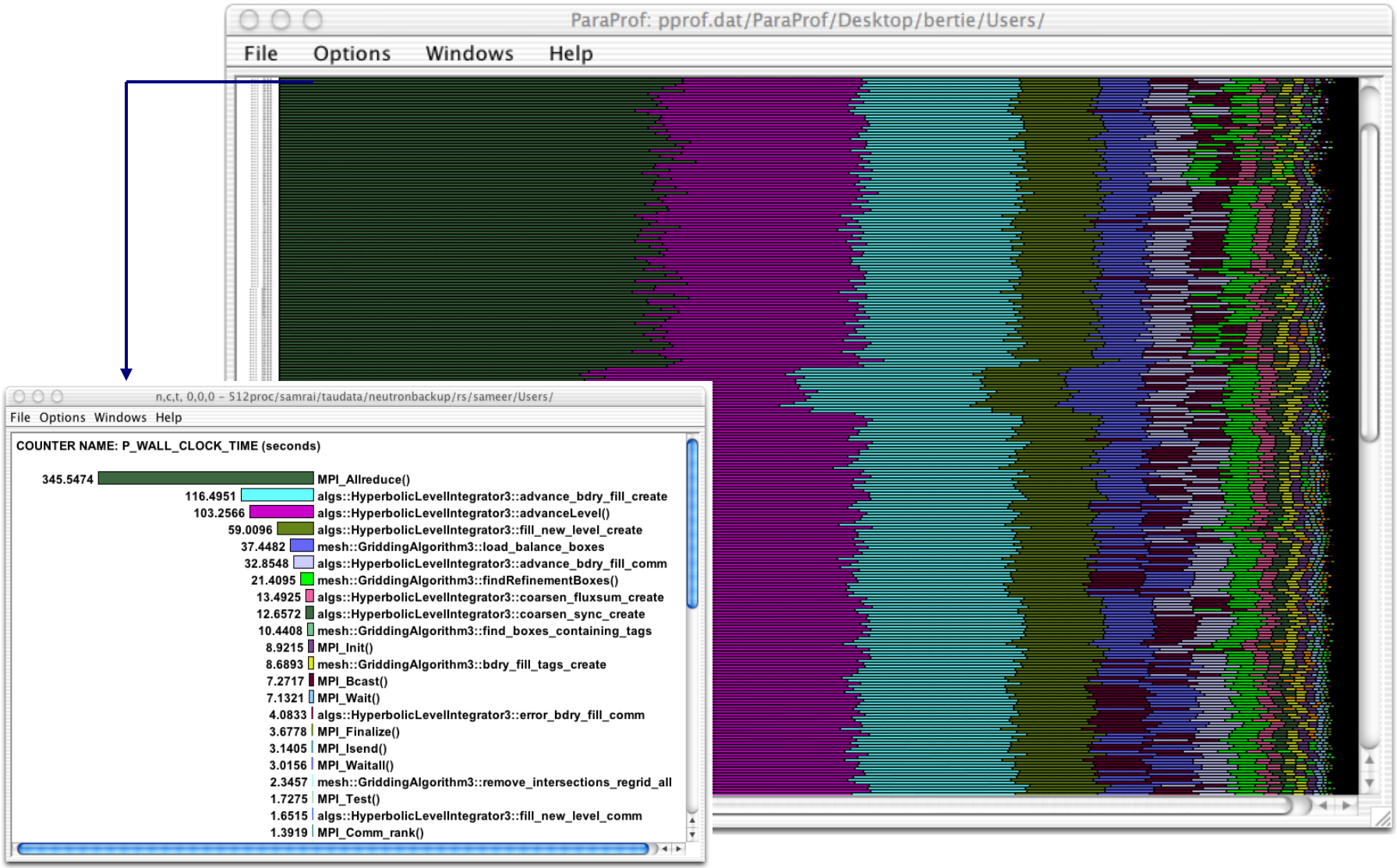


- Supports
  - Various profiling modes and tracing
  - Various forms of code instrumentation
  - C, C++, Fortran, Java, Python
  - MPI, multi-threading (OpenMP, Pthreads, …)
  - Accelerators

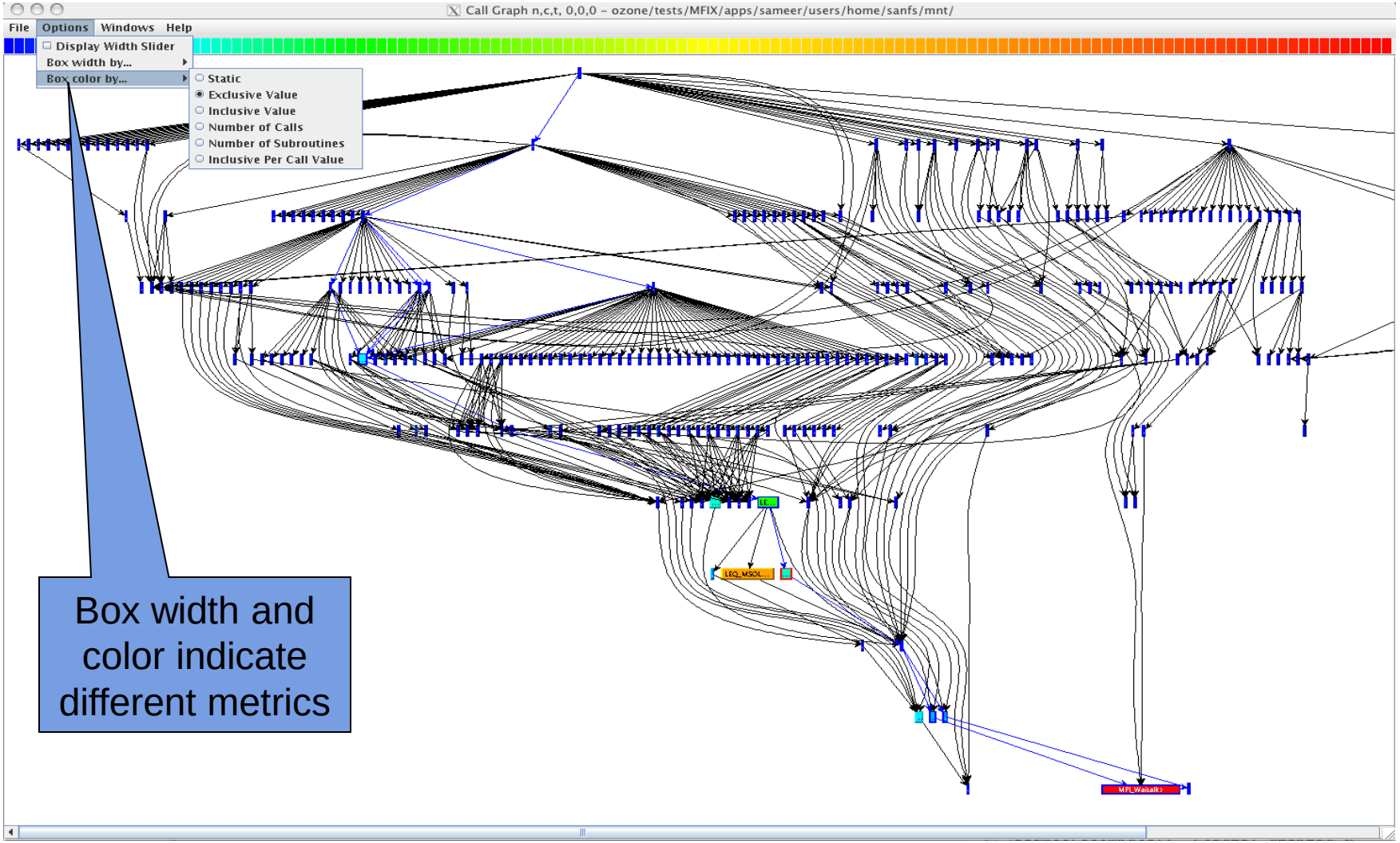
TAU: Instrumentation

- Flexible instrumentation mechanisms at multiple levels
  - Source code
    - manual
    - automatic
      - C, C++, F77/90/95 (Program Database Toolkit (PDT))
      - OpenMP (directive rewriting with Opari)
  - Object code
    - pre-instrumented libraries (e.g., MPI using PMPI)
    - statically-linked and dynamically-loaded (e.g., Python)
  - Executable code
    - dynamic instrumentation (pre-execution) (DynInst)
    - virtual machine instrumentation (e.g., Java using JVMPI)
- Support for performance mapping
- Support for object-oriented and generic programming

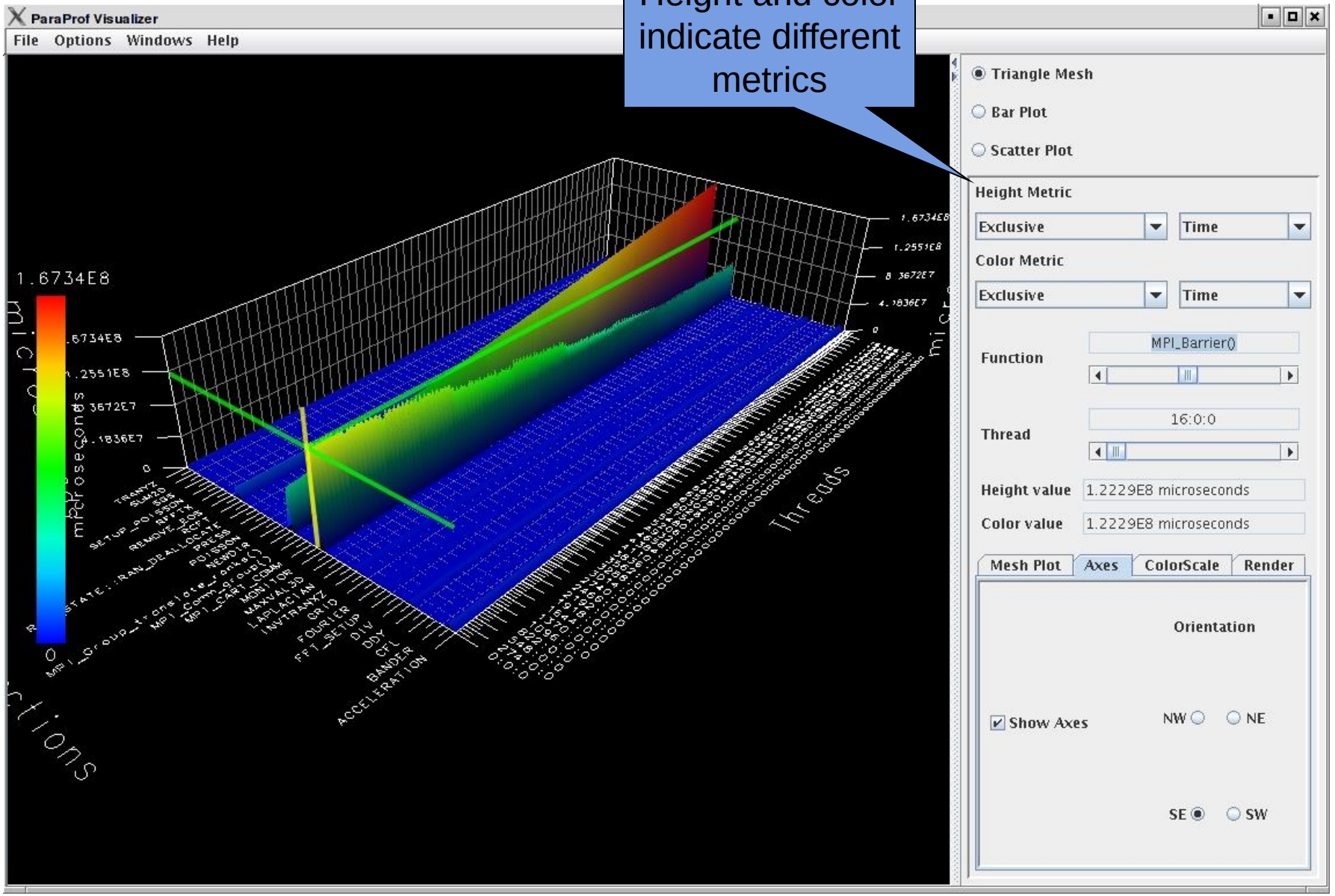
TAU: Basic Profile View



TAU: Callgraph Profile View



TAU: 3D Profile View



Documentation

- To check latest status
  - JUQUEEN: use “`module avail`”
  - JUROPATEST: use “`module spider`”

- Websites
  - http://www.fz-juelich.de/ias/jsc/juqueen/
  - http://www.fz-juelich.de/ias/jsc/juropatest/
    - User Info
      - Parallel Debugging ( )
      - Parallel Performance Analysis ( )
  - http://www.vi-hps.org/training/material/
    - Performance Tools LiveDVD image
    - Links to tool websites and documentation
    - Tutorial slides

Support

- For general support: sc@fz-juelich.de
- Tool-specific support via corresponding mailing lists
  - Score-P: support@score-p.org
  - Scalasca: scalasca@fz-juelich.de

- Workshops and Trainings:
  - Regular VI-HPS Tuning Workshops
    - Several days
    - Multiple tools, e.g. Score-P, Scalasca, Vampir, TAU, …
    - Bring-your-own-code
    - http://www.vi-hps.org/training/tws/
  - JUQUEEN Porting and Tuning Workshop Series

Mitglied der Helmholtz-Gemeinschaft

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FORSCHUNGSZENTRUM

Appendix

- Tool recipes

STAT: Recipe

- Compile and link your program with debug option: `-g`
- Load modules

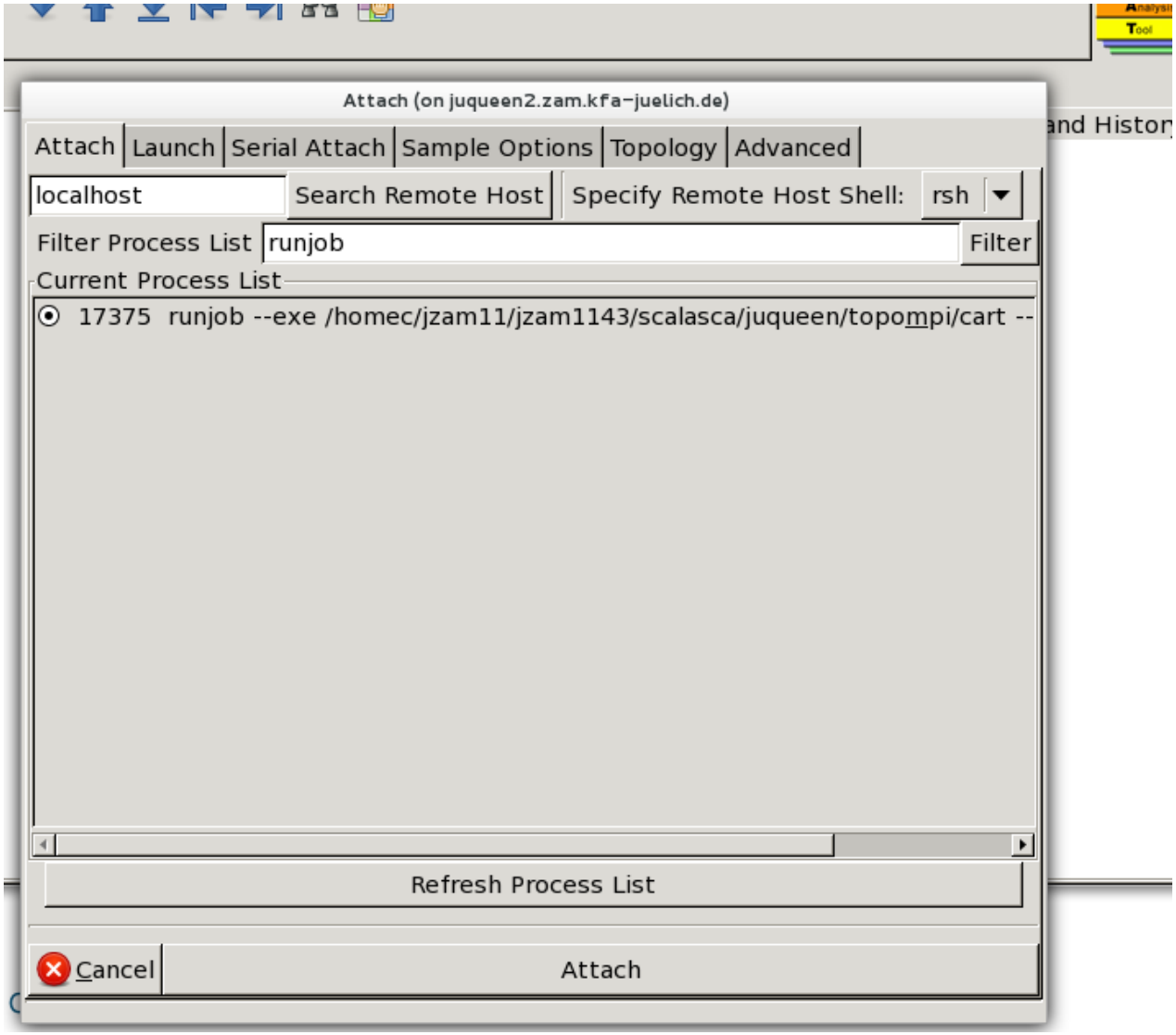
```
% ssh -X user@juqueen
[...]
juqueen% module load UNITE stat
UNITE loaded
stat/2.1 loaded
juqueen% STATGUI
```

- Submit job and attach to it from GUI
- **CAVEAT:**
  - Job needs to be started by login node where GUI is running
  - Add the following entry to the submission script

    `#@ requirements = (Machine == "juqueen<n>")`

    with <n> being the login node id

STAT: Attaching to a Job



TotalView: Recipe for JUQUEEN

- Compile and link your program with debug option: `-g`
- Use absolute paths for source code info: `-qfullpath`
- In case of optimized codes (XL), keep function call parameters: `-qkeepparm`
- Load modules

```
% ssh -X user@juqueen
[...]
juqueen% module load UNITE totalview
UNITE loaded
totalview/8.14.0-16-mrnet loaded

juqueen% mpixlcxx hello.cpp -qfullpath -qkeepparm -g -o helloworld
juqueen%
```

TotalView: Interactive Startup

- Interactively: call the `ltv` script
  - Creates a LoadLeveler batch script with required TotalView parameters
- If user cancels the script, it cancels the debugging job (does not eat your computing quota)

- **NOTE:**
  - License limited to 2048 MPI ranks (shared between all users)
  - Attaching to subset is recommended

TotalView: lltv Launch Script

```
% lltv -n <nodes> : -default_parallel_attach_subset=\
<rank-range> runjob -a --exe <program> -p <num>
```

- Starts <program> with <nodes> and <num> processes per node, attaches to <rank-range>:
  - Rank: that rank only
  - RankX-RankZ: all ranks, both inclusive
  - RankX-RankZ:stride every *stride*th between RankX and RankZ
- Example:

```
% lltv -n 2 : -default_parallel_attach_subset=\
2-6 runjob -a --exe helloworld -p 64

Creating LoadLeveler Job
Submitting LoadLeveler Interactive Job for Totalview
 Wait for job juqueen1c1.32768.0 to be started:.....
```

TotalView: Execution Recipe

- TotalView tries to debug “runjob” and shows no source code
  - Ignore it and press “GO”

- After some seconds, TotalView will detect parallel execution and ask if it should stop. Yes, it should stop.
- To find the correct point file/function to debug, use the “File-Open” command.
- Set your breakpoints, and press “GO” again. Debugging session will then start.

- To see a variable’s contents, double click on it in the source.

Vampir: Recipe (JUQUEEN)

1. `module load UNITE vampirserver`

2. Start Vampir server component (on frontend) using "`vampirserver start smp`"
   - Check output for port and pid

3. Connect to server from remote machine (see next slide) and analyze the trace

4. `vampirserver stop <pid>`
   - See above (2.)

Vampir: Recipe (local system)

1. Open SSH tunnel to JUQUEEN using
   "`ssh -L30000:localhost:<port> juqueen<n>`"

2. Start Vampir client component
   - For example: "`/usr/local/zam/unite/bin/vampir`"

3. Select
   1. "Open other…"
   2. "Remote file"
   3. "Connect" (keep defaults)
   4. File "`traces.otf2`" from Score-P trace measurement directory

HPCToolkit: Recipe

1. Compile your code with "`-g -qnoipa`"
   - For MPI, also make sure your application calls MPI_Comm_rank first on MPI_COMM_WORLD
2. Prefix your ***link command*** with "`hpclink`"
   - Ignore potential linker warnings ;-)
3. Run your application as usual, specifying requested metrics with sampling intervals in environment variable
   "`HPCRUN_EVENT_LIST`"
4. Perform static binary analysis with
   "`hpcstruct --loop-fwd-subst=no <app>`"
5. Combine measurements with
   "`hpcprof -S <struct file> \`
   `-I "<path_to_src>/*" <measurement_dir>`"
6. View results with
   "`hpcviewer <hpct_database>`"

TAU: Recipe

1. `Load TAU module#` once per session

   - `module load UNITE tau`

1. Specify programming model by setting `TAU_MAKEFILE` to one of `$TAU_MF_DIR/Makefile.tau-*`
2. Compile and link with
   - `tau_cc.sh file.c ...`
   - `tau_cxx.sh file.cxx...`
   - `tau_f90.sh file.f90 ...`
3. Execute with real input data
   Environment variables control measurement mode
   - TAU_PROFILE, TAU_TRACE, TAU_CALLPATH, …
4. Examine results with `paraprof`